EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	2337	((546/143) or (514/307) or (546/141) or (514/307)).CCLS.	US-PGPUB; USPAT	OR	OFF	2007/09/20 03:29
L2	393	1 and isoquinoline and potassium and inhibitors	US-PGPUB; USPAT	OR	OFF	2007/09/20 03:30

10572342

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1612bxr

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	JUL 02	LMEDLINE coverage updated
NEWS 3	JUL 02	SCISEARCH enhanced with complete author names
NEWS 4	JUL 02	CHEMCATS accession numbers revised
NEWS 5	JUL 02	CA/CAplus enhanced with utility model patents from China
NEWS 6	JUL 16	CAplus enhanced with French and German abstracts
NEWS 7	JUL 18	CA/CAplus patent coverage enhanced
NEWS 8	JUL 26	USPATFULL/USPAT2 enhanced with IPC reclassification
NEWS 9	JUL 30	USGENE now available on STN
NEWS 10	AUG 06	CAS REGISTRY enhanced with new experimental property tags
NEWS 11	AUG 06	BEILSTEIN updated with new compounds
NEWS 12	AUG 06	FSTA enhanced with new thesaurus edition
NEWS 13	AUG 13	CA/CAplus enhanced with additional kind codes for granted patents
NEWS 14	AUG 20	CA/CAplus enhanced with CAS indexing in pre-1907 records
NEWS 15	AUG 27	Full-text patent databases enhanced with predefined patent family display formats from INPADOCDB
NEWS 16	AUG 27	USPATOLD now available on STN
NEWS 17	AUG 28	CAS REGISTRY enhanced with additional experimental spectral property data
NEWS 18	SEP 07	STN AnaVist, Version 2.0, now available with Derwent World Patents Index
NEWS 19	SEP 13	FORIS renamed to SOFIS
NEWS 20	SEP 13	INPADOCDB enhanced with monthly SDI frequency
NEWS 21	SEP 17	CA/CAplus enhanced with printed CA page images from 1967-1998
NEWS 22	SEP 17	CAplus coverage extended to include traditional medicine patents

NEWS EXPRESS 19 SEPTEMBER 2007: CURRENT WINDOWS VERSION IS V8.2, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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Updated Search

10572342

of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 01:26:17 ON 20 SEP 2007

=> file reg
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 01:26:30 ON 20 SEP 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 18 SEP 2007 HIGHEST RN 947490-11-1
DICTIONARY FILE UPDATES: 18 SEP 2007 HIGHEST RN 947490-11-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

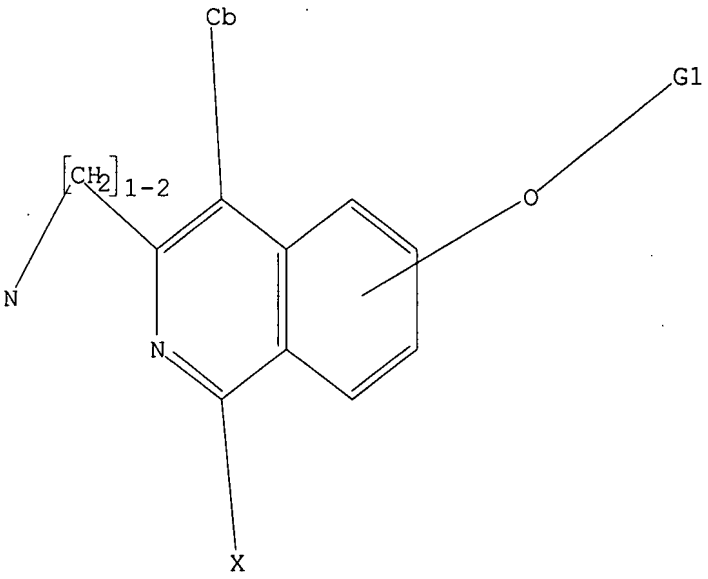
=>
Uploading C:\Documents and Settings\brobinson1\My Documents\stnweb\Queries\ftgh.str

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR

Updated Search

10572342



G1 Me,Et

Structure attributes must be viewed using STN Express query preparation.

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=> s l1
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SAMPLE SCREEN SEARCH COMPLETED -        7 TO ITERATE

100.0% PROCESSED         7 ITERATIONS                                  0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:            7 TO      298
PROJECTED ANSWERS:               0 TO        0

L2             0 SEA SSS SAM L1

=> s l1 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 171.65 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 01:29:14 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      103 TO ITERATE

100.0% PROCESSED       103 ITERATIONS                                 1 ANSWERS
SEARCH TIME: 00.00.01

L3             1 SEA SSS FUL L1

=> file hcaplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                              173.90     174.11

FILE 'HCAPLUS' ENTERED AT 01:29:18 ON 20 SEP 2007
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Updated Search

10572342

FILE COVERS 1907 - 20 Sep 2007 VOL 147 ISS 13
FILE LAST UPDATED: 18 Sep 2007 (20070918/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3
L4 1 L3

=> d l4, ibib abs hitstr, 1

L4 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:300191 HCAPLUS
DOCUMENT NUMBER: 142:373697
TITLE: Preparation of isoquinoline derivatives as potassium channel inhibitors
INVENTOR(S): Trotter, B. Wesley; Nanda, Kausik K.; Kett, Nathan R.; Dinsmore, Christopher J.; Ponticello, Gerald S.; Claremon, David A.
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 115 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005030130	A2	20050407	WO 2004-US30486	20040917
WO 2005030130	A3	20060119		

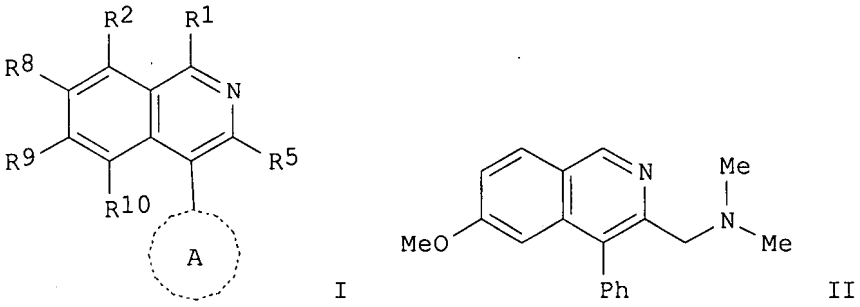
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

Updated Search

10572342

AU 2004275720	A1	20050407	AU 2004-275720		20040917
CA 2539479	A1	20050407	CA 2004-2539479		20040917
EP 1667979	A2	20060614	EP 2004-784370		20040917
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR					
CN 1856475	A	20061101	CN 2004-80027385		20040917
JP 2007506743	T	20070322	JP 2006-528072		20040917
IN 2006DN00877	A	20070810	IN 2006-DN877		20060220
US 2006276450	A1	20061207	US 2006-572342		20060317
PRIORITY APPLN. INFO.:			US 2003-505143P	P	20030923
			WO 2004-US30486	W	20040917

OTHER SOURCE(S): MARPAT 142:373697
GI



AB Title compds. represented by the formula I [wherein ring A = (un)substituted (hetero)aryl or heterocyclic ring; R1 = H, CN, halo, (alkyl)amino, etc.; R2, R8-R10 = independently H, halo, aminocarbamoyl, etc.; R5 = H, halo, (cyclo)alkyl, etc.; and pharmaceutically acceptable salts, crystal forms or hydrates thereof] were prepared as potassium channel inhibitors. For example, Ni-catalyzed reduction of 1-chloro-6-methoxy-4-phenylisoquinoline-3-carbonitrile and followed by condensation with formaldehyde, gave II•2HCl. I provided ≥50% inhibition at concentration ≤33 μM in the high-throughput Kv1.5 planar patch clamp assay and ≥25% inhibition at concentration ≤25 μM in the AAS (atomic absorption spectroscopy) assay. Thus, I and their pharmaceutical compns. are useful as potassium channel inhibitors for the treatment of cardiac arrhythmias, and the like.

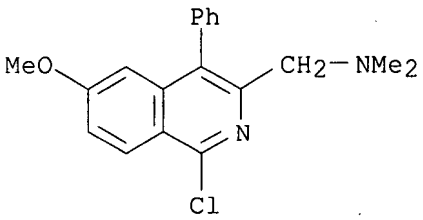
IT 849545-74-0P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of isoquinoline derivs. as potassium channel inhibitors)

RN 849545-74-0 HCAPLUS

CN 3-Isoquinolinemethanamine, 1-chloro-6-methoxy-N,N-dimethyl-4-phenyl- (9CI) (CA INDEX NAME)

Updated Search

10572342

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=> file caold
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     7.87     181.98

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                    -0.78      -0.78

FILE 'CAOLD' ENTERED AT 01:29:31 ON 20 SEP 2007
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FILE COVERS 1907-1966
FILE LAST UPDATED:  01 May 1997 (19970501/UP)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.  Title keywords, authors, patent
  assignees, and patent information, e.g., patent numbers, are
  now searchable from 1907-1966.  TIFF images of CA abstracts
  printed between 1907-1966 are available in the PAGE
  display formats.

  New CAS Information Use Policies, enter HELP USAGETERMS for details.

  This file supports REG1stRY for direct browsing and searching of
  all substance data from the REGISTRY file.  Enter HELP FIRST for
  more information.

=> d his

     (FILE 'HOME' ENTERED AT 01:26:17 ON 20 SEP 2007)

     FILE 'REGISTRY' ENTERED AT 01:26:30 ON 20 SEP 2007
L1              STRUCTURE UPLOADED
L2            0 S L1
L3            1 S L1 FULL

     FILE 'HCAPLUS' ENTERED AT 01:29:18 ON 20 SEP 2007
L4            1 S L3

     FILE 'CAOLD' ENTERED AT 01:29:31 ON 20 SEP 2007

=> s l3
L5            0 L3
```

Updated Search

10572342

```
=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.45     182.43

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                     0.00      -0.78

FILE 'REGISTRY' ENTERED AT 01:29:39 ON 20 SEP 2007
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provided by InfoChem.

STRUCTURE FILE UPDATES:   18 SEP 2007  HIGHEST RN 947490-11-1
DICTIONARY FILE UPDATES:  18 SEP 2007  HIGHEST RN 947490-11-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Documents and Settings\brobinson1\My Documents\stnweb\Queries\asdf.str

L6      STRUCTURE UPLOADED

=> d l6
L6 HAS NO ANSWERS
L6              STR
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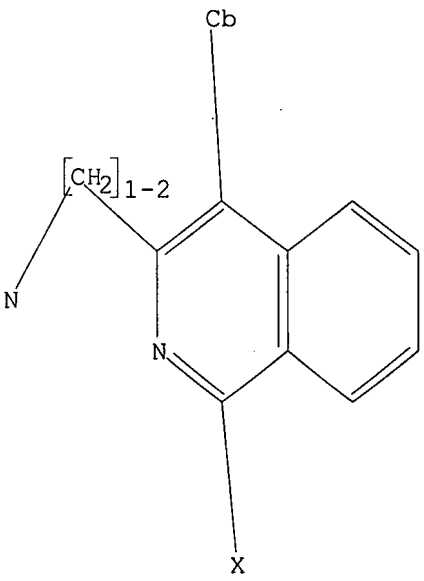
Updated Search

10572342



Structure attributes must be viewed using STN Express query preparation.

```
=> s l6
SAMPLE SEARCH INITIATED 01:31:04 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -       10 TO ITERATE

100.0% PROCESSED       10 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:           11 TO      389
PROJECTED ANSWERS:               0 TO        0

L7            0 SEA SSS SAM L6

=> s l6 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 171.65 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 01:31:09 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      122 TO ITERATE

100.0% PROCESSED      122 ITERATIONS                                1 ANSWERS
SEARCH TIME: 00.00.01

L8            1 SEA SSS FUL L6

=>
Uploading C:\Documents and Settings\brobinson1\My Documents\stnweb\Queries\asdfa.str

L9      STRUCTURE UPLOADED

=> s l9
SAMPLE SEARCH INITIATED 01:31:57 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      434 TO ITERATE
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Updated Search

10572342

100.0% PROCESSED 434 ITERATIONS 7 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 7431 TO 9929
PROJECTED ANSWERS: 7 TO 298

L10 7 SEA SSS SAM L9

=> s l9 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 171.65 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 01:32:01 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 8772 TO ITERATE

100.0% PROCESSED 8772 ITERATIONS 78 ANSWERS
SEARCH TIME: 00.00.01

L11 78 SEA SSS FUL L9

=> file hcaplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 345.10 527.53

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE ENTRY TOTAL SESSION
CA SUBSCRIBER PRICE 0.00 -0.78

FILE 'HCAPLUS' ENTERED AT 01:32:04 ON 20 SEP 2007
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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 20 Sep 2007 VOL 147 ISS 13
FILE LAST UPDATED: 18 Sep 2007 (20070918/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l11
L12 33 L11

=> s l12 and trotter, b?/au

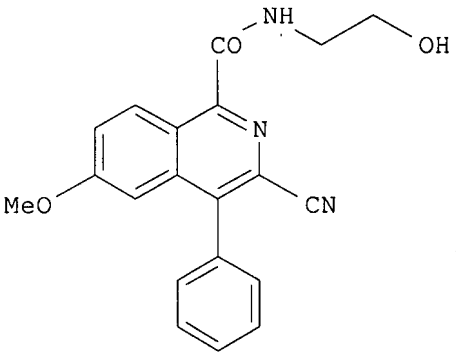
Updated Search

10572342

48 TROTTER, B?/AU
L13 2 L12 AND TROTTER, B?/AU

=> d l13, ibib abs hitstr, 1-2

L13 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:1252121 HCAPLUS
DOCUMENT NUMBER: 146:142484
TITLE: Design and Synthesis of Novel Isoquinoline-3-nitriles as Orally Bioavailable Kv1.5 Antagonists for the Treatment of Atrial Fibrillation
AUTHOR(S): Trotter, B. Wesley; Nanda, Kausik K.; Kett, Nathan R.; Regan, Christopher P.; Lynch, Joseph J.; Stump, Gary L.; Kiss, Laszlo; Wang, Jixin; Spencer, Robert H.; Kane, Stefanie A.; White, Rebecca B.; Zhang, Rena; Anderson, Kenneth D.; Liverton, Nigel J.; McIntyre, Charles J.; Beshore, Douglas C.; Hartman, George D.; Dinsmore, Christopher J.
CORPORATE SOURCE: Departments of Medicinal Chemistry, Stroke, and Neurodegeneration Automated Biotechnology Pain Research, and Drug Metabolism, Merck Research Laboratories, West Point, PA, 19486, USA
SOURCE: Journal of Medicinal Chemistry (2006), 49(24), 6954-6957
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 146:142484
GI

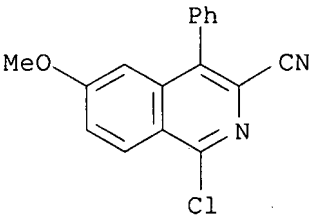


AB Novel 3-cyanoisoquinoline Kv1.5 antagonists have been prepared and evaluated in in vitro and in vivo assays for inhibition of the Kv1.5 potassium channel and its associated cardiac potassium current, IKur. Structural modifications of the isoquinolinone lead afforded compds. (e.g. I) with excellent potency, selectivity, and oral bioavailability.
IT 849546-10-7P 849546-48-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of isoquinoline-3-nitriles as orally bioavailable Kv1.5 antagonists for the treatment of atrial fibrillation)
RN 849546-10-7 HCAPLUS

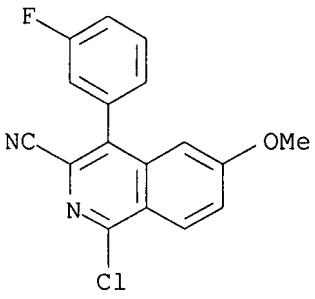
Updated Search

10572342

CN 3-Isoquinolinecarbonitrile, 1-chloro-6-methoxy-4-phenyl- (CA INDEX NAME)



RN 849546-48-1 HCAPLUS
CN 3-Isoquinolinecarbonitrile, 1-chloro-4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:300191 HCAPLUS
DOCUMENT NUMBER: 142:373697
TITLE: Preparation of isoquinoline derivatives as potassium channel inhibitors
INVENTOR(S): Trotter, B. Wesley; Nanda, Kausik K.; Kett, Nathan R.; Dinsmore, Christopher J.; Ponticello, Gerald S.; Claremon, David A.
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 115 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005030130	A2	20050407	WO 2004-US30486	20040917
WO 2005030130	A3	20060119		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

Updated Search

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2004275720	A1	20050407	AU 2004-275720		20040917
CA 2539479	A1	20050407	CA 2004-2539479		20040917
EP 1667979	A2	20060614	EP 2004-784370		20040917
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR					
CN 1856475	A	20061101	CN 2004-80027385		20040917
JP 2007506743	T	20070322	JP 2006-528072		20040917
IN 2006DN00877	A	20070810	IN 2006-DN877		20060220
US 2006276450	A1	20061207	US 2006-572342		20060317
PRIORITY APPLN. INFO.:			US 2003-505143P	P	20030923
			WO 2004-US30486	W	20040917

OTHER SOURCE(S): MARPAT 142:373697

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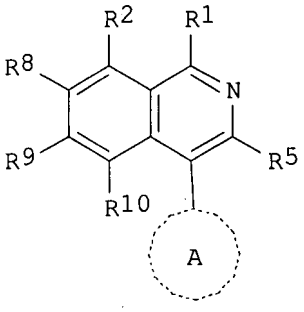
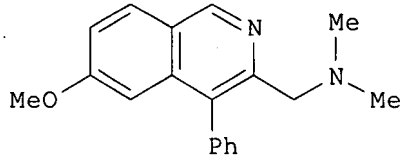


I



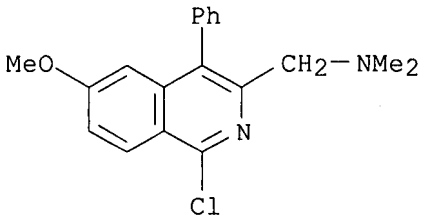
II

AB Title compds. represented by the formula I [wherein ring A = (un)substituted (hetero)aryl or heterocyclic ring; R1 = H, CN, halo, (alkyl)amino, etc.; R2, R8-R10 = independently H, halo, aminocarbamoyl, etc.; R5 = H, halo, (cyclo)alkyl, etc.; and pharmaceutically acceptable salts, crystal forms or hydrates thereof] were prepared as potassium channel inhibitors. For example, Ni-catalyzed reduction of 1-chloro-6-methoxy-4-phenylisoquinoline-3-carbonitrile and followed by condensation with formaldehyde, gave II•2HCl. I provided ≥50% inhibition at concentration ≤33 μM in the high-throughput Kv1.5 planar patch clamp assay and ≥25% inhibition at concentration ≤25 μM in the AAS (atomic absorption spectroscopy) assay. Thus, I and their pharmaceutical compns. are useful as potassium channel inhibitors for the treatment of cardiac arrhythmias, and the like.

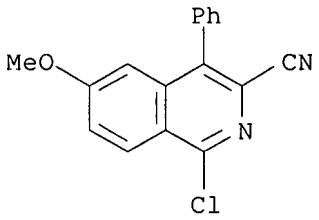
IT 849545-74-0P 849546-10-7P 849546-48-1P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of isoquinoline derivs. as potassium channel inhibitors)

RN 849545-74-0 HCAPLUS

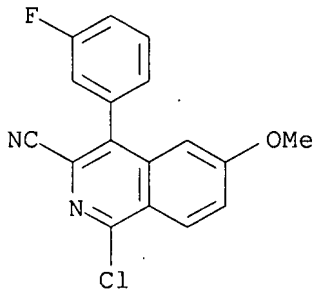
CN 3-Isoquinolinemethanamine, 1-chloro-6-methoxy-N,N-dimethyl-4-phenyl- (9CI) (CA INDEX NAME)



RN 849546-10-7 HCAPLUS
CN 3-Isoquinolinecarbonitrile, 1-chloro-6-methoxy-4-phenyl- (CA INDEX NAME)

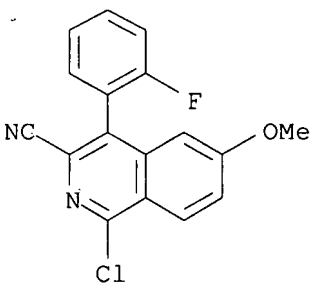


RN 849546-48-1 HCAPLUS
CN 3-Isoquinolinecarbonitrile, 1-chloro-4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)

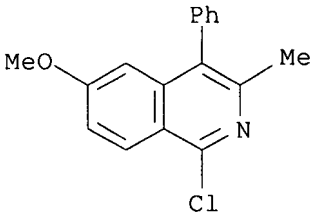


IT 849547-01-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of isoquinoline derivs. as potassium channel inhibitors)
RN 849547-01-9 HCAPLUS
CN 3-Isoquinolinecarbonitrile, 1-chloro-4-(2-fluorophenyl)-6-methoxy- (9CI) (CA INDEX NAME)

10572342



IT 849548-90-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of isoquinoline derivs. as potassium channel inhibitors)
RN 849548-90-9 HCAPLUS
CN Isoquinoline, 1-chloro-6-methoxy-3-methyl-4-phenyl- (9CI) (CA INDEX NAME)



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FILE 'REGISTRY' ENTERED AT 01:26:30 ON 20 SEP 2007
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L2 0 S L1
L3 1 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 01:29:18 ON 20 SEP 2007
L4 1 S L3

FILE 'CAOLD' ENTERED AT 01:29:31 ON 20 SEP 2007
L5 0 S L3

FILE 'REGISTRY' ENTERED AT 01:29:39 ON 20 SEP 2007
L6 STRUCTURE UPLOADED
L7 0 S L6
L8 1 S L6 FULL
L9 STRUCTURE UPLOADED
L10 7 S L9
L11 78 S L9 FULL

FILE 'HCAPLUS' ENTERED AT 01:32:04 ON 20 SEP 2007
L12 33 S L11
L13 2 S L12 AND TROTTER, B?/AU

Updated Search

10572342

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L17          0 L14 AND DINSMORE, C?/AU

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L18          0 L14 AND PONTICELLO, G?/AU

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           140 CLAREMON, D?/AU
L19          0 L14 AND CLAREMON, D?/AU

=> d l14, ibib abs hitstr, 1-31

L14  ANSWER 1 OF 31  HCAPLUS  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:         2007:410660  HCAPLUS
DOCUMENT NUMBER:          146:421855
TITLE:                    Preparation of 1-aminoisoquinoline derivatives as
                          melanin concentrating receptor (MCH), particularly
                          MCH-1R, antagonists
INVENTOR(S):              Augereau, Jean Michel; Courtemanche, Gilles; Geslin,
                          Michel
PATENT ASSIGNEE(S):       Sanofi Aventis, Fr.
SOURCE:                   Fr. Demande, 34pp.
                          CODEN: FRXXBL
DOCUMENT TYPE:            Patent
LANGUAGE:                 French
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.         DATE
     ---------------      ----   --------    --------------------    --------
     FR 2891825            A1    20070413    FR 2005-10410           20051012
     WO 2007042668         A1    20070419    WO 2006-FR2285          20061011
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP,
             KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN,
             MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS,
             RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ,
             UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
             CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
             GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM
PRIORITY APPLN. INFO.:                       FR 2005-10410       A  20051012
OTHER SOURCE(S):          MARPAT 146:421855
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Updated Search

10572342

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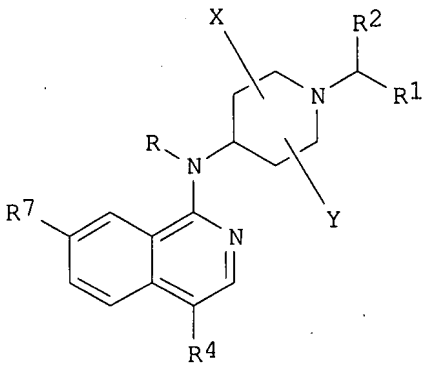

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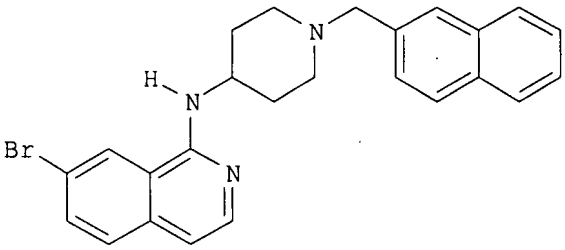

II

AB Title compds. I [R = H, cyclo/fluoro/alkyl, CH2C.tplbond.CH, etc.; R1 = (un)substituted (hetero)aryl; R2 = H, alkyl; R4 = H, alkyl, (un)substituted heterocyclyl, (hetero)aryl, etc.; R7 = H, halo, alkyl, alkoxy, CO2H, CN, NH2 and derivs., etc.; X, Y = independently H, alkyl; or X and Y are joined by a single bond, or an alkylene group; and their acid addition salts, and their hydrates and solvates, and their enantiomers, diastereomers, and their mixts.] were prepared as melanin concentrating receptor (MCH), particularly MCH-1R, antagonists. Thus, amination of 7-bromo-1-chloroisoquinoline with N-[1-[(2-naphthyl)methyl]piperidin-4-yl]amine and acidulation of the aminoisoquinoline with HCl gave II•2HCl. I displayed IC50's < 1 μM in a radioligand assay for MCH-1R. I are MCH-1R antagonists, and their compns. are useful for treating obesity, metabolic disorders, anxiety, depression, etc. (no data).

IT 934265-05-1P, 1-Chloro-4-(4-chlorophenyl)-7-methoxyisoquinoline
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of 1-aminoisoquinoline derivs. as melanin concentrating receptor 1 antagonists)

RN 934265-05-1 HCAPLUS

CN Isoquinoline, 1-chloro-4-(4-chlorophenyl)-7-methoxy- (CA INDEX NAME)

Updated Search

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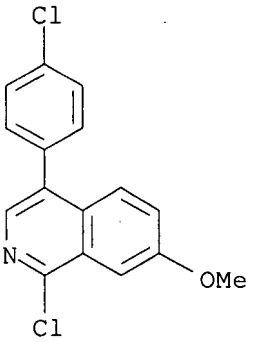


REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 2 OF 31 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:978927 HCAPLUS
DOCUMENT NUMBER: 145:348613
TITLE: Methods of screening for agents for the treatment of postmenopausal vulvovaginal atrophy by analysis of effects on marker gene expression
INVENTOR(S): Crabtree, Judy Sue; Harris, Heather Anne; Jelinsky, Scott Alan; Zhang, Xiaochun; Peano, Bryan John
PATENT ASSIGNEE(S): Wyeth, John, and Brother Ltd., USA
SOURCE: PCT Int. Appl., 109pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006099610	A2	20060921	WO 2006-US9995	20060316
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
US 2006216295	A1	20060928	US 2006-377756	20060316
PRIORITY APPLN. INFO.:			US 2005-662663P P	20050317
			US 2005-688946P P	20050609

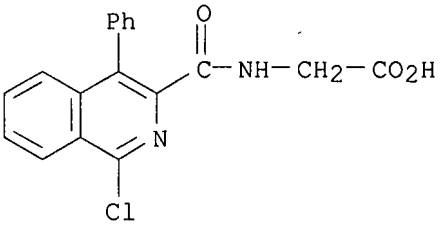
OTHER SOURCE(S): MARPAT 145:348613
AB Methods for the identification of effector mols. useful in the treatment of vulvovaginal atrophy by anal. of their effects on the expression of atrophy-related genes is described. Methods of treating vulvovaginal atrophy comprising administering the effector mols. are also disclosed.
IT 808118-15-2D, salts, esters, prodrugs
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(for treatment of vulvovaginal atrophy; methods of screening for agents

Updated Search

for treatment of postmenopausal vulvovaginal atrophy by anal. of effects on marker gene expression)

RN 808118-15-2 HCAPLUS

CN Glycine, N-[(1-chloro-4-phenyl-3-isoquinolinyl)carbonyl]- (9CI) (CA INDEX NAME)



L14 ANSWER 3 OF 31 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:1080867 HCAPLUS

DOCUMENT NUMBER: 142:56195

TITLE: Preparation of isoquinolinecarboxamides and their use in mediating hypoxia inducible factor and increasing endogenous erythropoietin

INVENTOR(S): Arend, Michael P.; Flippin, Lee A.; Guenzler-Pukall, Volkmar; Ho, Wen-Bin; Turtle, Eric D.; Du, Xiaohui

PATENT ASSIGNEE(S): Fibrogen, Inc., USA

SOURCE: PCT Int. Appl., 302 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004108681	A1	20041216	WO 2004-US17773	20040604
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004245552	A1	20041216	AU 2004-245552	20040604
CA 2528232	A1	20041216	CA 2004-2528232	20040604
US 2004254215	A1	20041216	US 2004-861082	20040604
EP 1644336	A1	20060412	EP 2004-754384	20040604
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
BR 2004011055	A	20060725	BR 2004-11055	20040604
CN 1816527	A	20060809	CN 2004-80015559	20040604
JP 2006527200	T	20061130	JP 2006-515202	20040604
IN 2005KN02370	A	20061013	IN 2005-KN2370	20051124
MX 2005PA13116	A	20060720	MX 2005-PA13116	20051205

Updated Search

10572342

NO 2006000024	A	20060130	NO 2006-24		20060103
US 2006217416	A1	20060928	US 2006-442727		20060526
US 2007155784	A1	20070705	US 2006-549571		20061013
US 2007185159	A1	20070809	US 2007-624949		20070119
PRIORITY APPLN. INFO.:			US 2003-476420P	P	20030606
			US 2003-476519P	P	20030606
			US 2003-476633P	P	20030606
			US 2003-476811P	P	20030606
			US 2004-861082	A1	20040604
			WO 2004-US17773	W	20040604

OTHER SOURCE(S): MARPAT 142:56195

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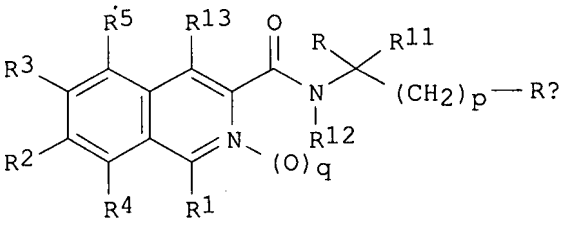

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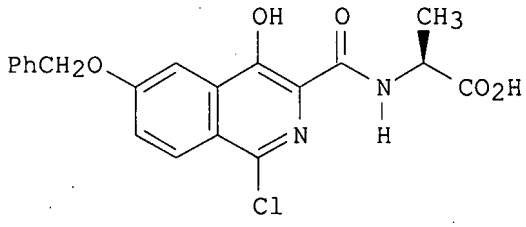


II

AB Title compds. I [wherein q = 0 or 1; p = 0 or 1; Ra = COOH or -WR8; W = O, S(O)n or NR9; R8, R9 = H, (un)substituted alkyl or (hetero)aryl; n = 0-2; R1 = H, (un)substituted alk(yl/oxy), amino or sulf(a/i/o)nyl; R2, R3 = H, (un)substituted alk(yl/oxy), (hetero)aryl, aryloxy, sulf(a/i/o)nyl, halo, OH or cyano; R4, R5 = H, halo, (un)substituted alk(yl/oxy) or (hetero)aryl, R = H, D or Me; R11 = H, D or (un)substituted alkyl; R12 = H or alkyl; R13 = H, (un)substituted (cyclo)alkoxy or aryloxy; et al., with some limitations, and pharmaceutically acceptable salts, esters and prodrugs thereof] were prepared For example, 6-benzyloxy-1-chloro-4-hydroxyisoquinoline-3-carboxylic acid underwent HATU-mediated coupling reaction with L-alanine Me ester hydrochloride followed by basic hydrolysis to give compound II. I were reported to be active in several biol. assays (no data). Compds. I and their pharmaceutical compns. are useful in mediating hypoxia inducible factor (HIF) and in treating erythropoietin-associated conditions, such as anemic and neurol. disorders, by increasing endogenous erythropoietin.

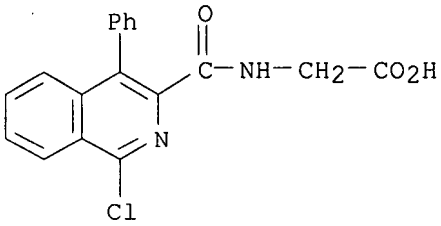
IT 808118-15-2P, [[(1-Chloro-4-phenylisoquinolin-3-yl)carbonyl]amino]acetic acid
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of isoquinolinecarboxamides as modulators of hypoxia inducible factor and endogenous erythropoietin)

RN 808118-15-2 HCAPLUS

Updated Search

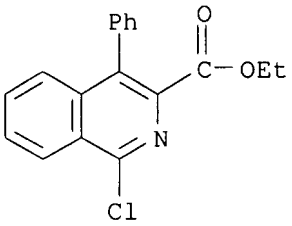
10572342

CN Glycine, N-[(1-chloro-4-phenyl-3-isoquinolinyl)carbonyl]- (9CI) (CA INDEX NAME)

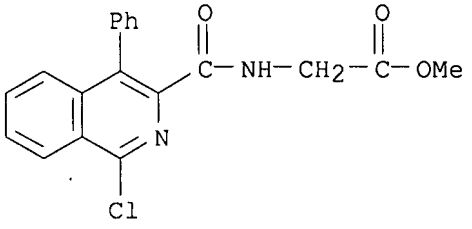


IT 808118-13-0P, 1-Chloro-4-phenylisoquinoline-3-carboxylic acid ethyl ester 808118-14-1P, [[(1-Chloro-4-phenylisoquinolin-3-yl)carbonyl]amino]acetic acid methyl ester
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of isoquinolinecarboxamides as modulators of hypoxia inducible factor and endogenous erythropoietin)

RN 808118-13-0 HCAPLUS
CN 3-Isoquinolinecarboxylic acid, 1-chloro-4-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



RN 808118-14-1 HCAPLUS
CN Glycine, N-[(1-chloro-4-phenyl-3-isoquinolinyl)carbonyl]-, methyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

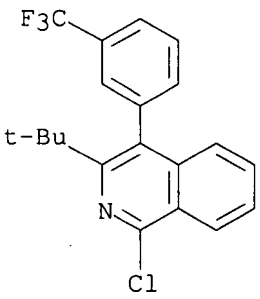
L14 ANSWER 4 OF 31 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:906475 HCAPLUS
DOCUMENT NUMBER: 140:106853
TITLE: Predicting the Genotoxicity of Polycyclic Aromatic Compounds from Molecular Structure with Different

Updated Search

10572342

Classifiers

AUTHOR(S): He, Linnan; Jurs, Peter C.; Custer, Laura L.; Durham, Stephen K.; Pearl, Greg M.
CORPORATE SOURCE: Department of Chemistry, The Pennsylvania State University, University Park, PA, 16802, USA
SOURCE: Chemical Research in Toxicology (2003), 16(12), 1567-1580
CODEN: CRTOEC; ISSN: 0893-228X
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Classification models were developed to provide accurate prediction of genotoxicity of 277 polycyclic aromatic compds. (PACs) directly from their mol. structures. Numerical descriptors encoding the topol., geometric, electronic, and polar surface area properties of the compds. were calculated to represent the structural information. Each compound's genotoxicity was represented with IMAX (maximal SOS induction factor) values measured by the SOS Chromotest in the presence and absence of S9 rat liver homogenate. The compds.' class identity was determined by a cutoff IMAX value of 1.25-compds. with IMAX > 1.25 in either test were classified as genotoxic, and the ones with IMAX ≤ 1.25 were nongenotoxic. Several binary classification models were generated to predict genotoxicity: k-nearest neighbor (k-NN), linear discriminant anal., and probabilistic neural network. The study showed k-NN to provide the highest predictive ability among the three classifiers with a training set classification rate of 93.5%. A consensus model was also developed that incorporated the three classifiers and correctly predicted 81.2% of the 277 compds. It also provided a higher prediction rate on the genotoxic class than any other single model.
IT 195512-04-0, 3-tert-Butyl-1-chloro-4-[3-(trifluoromethyl)phenyl]isoquinoline
RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL (Biological study)
(predicting genotoxicity of polycyclic aromatic compds. from mol. structure with different classifiers)
RN 195512-04-0 HCAPLUS
CN Isoquinoline, 1-chloro-3-(1,1-dimethylethyl)-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 5 OF 31 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:670166 HCAPLUS
DOCUMENT NUMBER: 138:153423
TITLE: Design, syntheses and biological evaluations of

10572342

nonpeptidic caspase 3 inhibitors

AUTHOR(S): Kim, Eun-sook; Yoo, Sung-eun; Yi, Kyu Yang; Lee, Sunkyung; Noh, Jae-sung; Jung, Yong-Sam; Kim, Eunhee; Jeong, Nakcheol

CORPORATE SOURCE: Department of Chemistry, Division of Chemistry and Molecular Engineering, Korea University, Seoul, 136-701, S. Korea

SOURCE: Bulletin of the Korean Chemical Society (2002), 23(7), 1003-1010
CODEN: BKCSDE; ISSN: 0253-2964

PUBLISHER: Korean Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:153423

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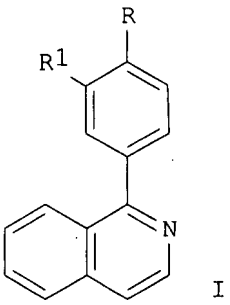


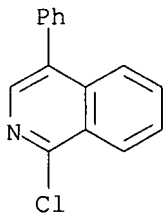
I

AB Novel caspase 3 inhibitors were designed , based on the active sites of the enzyme and their inhibitory activity was evaluated. The arylisoquinolines (I, R = OMe, R1 = H; R = H, R1 = OMe), their N-oxides, and the methiodide of I [R = OMe, R1 = H] showed significant inhibitory effects (>50%).

IT 65810-96-0P, 1-(4-Chlorophenyl)isoquinoline
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation of aryl-, arylcarbamoyl-, and aryloxyisoquinolines as caspase 3 inhibitors)

RN 65810-96-0 HCAPLUS

CN Isoquinoline, 1-chloro-4-phenyl- (6CI, 9CI) (CA INDEX NAME)



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

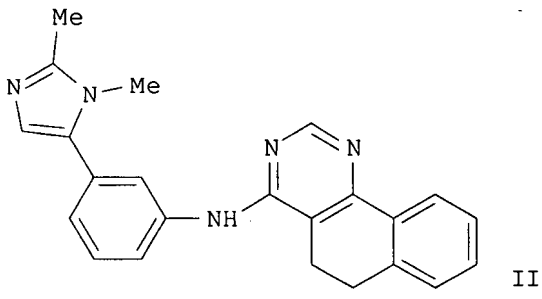
Updated Search

10572342

L14 ANSWER 6 OF 31 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:851122 HCAPLUS
DOCUMENT NUMBER: 135:371759
TITLE: Preparation of N-imidazolylphenyl-5,6-dihydrobenzo[h]quinazolin-4-amines and other N-containing heterocyclic amines as 5-hydroxytryptamine antagonists for treatment of CNS disorders
INVENTOR(S): Yamada, Akira; Spears, Glen; Hayashida, Hisashi; Tomishima, Masaki; Ito, Kiyotaka; Imanishi, Masashi
PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 154 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2001087845	A2	20011122	WO 2001-JP4002		20010514
WO 2001087845	A3	20020829			
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
AU 2001056728	A5	20011126	AU 2001-56728		20010514
US 2003176454	A1	20030918	US 2002-258582		20021101
PRIORITY APPLN. INFO.:			AU 2000-7501	A	20000515
			AU 2000-1955	A	20001207
			WO 2001-JP4002	W	20010514

OTHER SOURCE(S): MARPAT 135:371759
GI



II

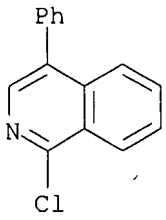
AB Title compds. AMQNHZ [I; wherein A = H, (un)substituted, unsatd., N-containing heterocyclic group, or C(NH)NHR; R = (un)substituted aryl or heterocyclic group; M = (CH2)n, (CH2)nO(CH2)m, or (CH2)nNH(CH2)m; n and m = independently 0-2; Q = (un)substituted cycloalkylene group, arylene, or

Updated Search

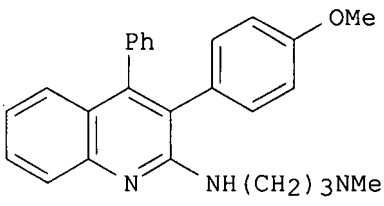
divalent heterocyclic group; Z = (un)substituted, unsatd., mono-, di-, tri-, or tetra-cyclic, N-containing heterocyclic group which may contain addnl. N, O, and S atoms as the ring member(s), e.g. indeno[1,2,3-de]phthalazinyl or 5,6-dihydrobenzo[h]quinazolinyl; and the prodrugs or pharmaceutically acceptable salts thereof] were prepared For example, a mixture of 4-chloro-5,6-dihydrobenzo[h]quinazoline, 3-(1,2-dimethyl-1H-imidazol-5-yl)aniline, and 1,3-dimethyl-2-imidazolidinone was heated for an hour at 200°C, cooled, treated with 1N aqueous NaOH and water, and worked up to give II. I are 5-hydroxytryptamine (5-HT) antagonists useful for the prevention and/or treatment of central nervous system (CNS) disorders, such as anxiety, depression, obsessive compulsive disorders, migraine, anorexia, Alzheimer's disease, sleep disorders, bulimia, panic attacks, withdrawal from drug abuse, schizophrenia, and disorders associated with spinal trauma and/or head injury (no data).

IT 65810-96-0P, 1-Chloro-4-phenylisoquinoline
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of N-(imidazolylphenyl)dihydrobenzo[h]quinazolinamines and other N-containing heterocyclic amines as 5-hydroxytryptamine antagonists for treatment of CNS disorders)

RN 65810-96-0 HCAPLUS
CN Isoquinoline, 1-chloro-4-phenyl- (6CI, 9CI) (CA INDEX NAME)



L14 ANSWER 7 OF 31 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:840672 HCAPLUS
DOCUMENT NUMBER: 134:100750
TITLE: Diphenyl quinolines and isoquinolines: synthesis and primary biological evaluation
AUTHOR(S): Croisy-Delcey, Martine; Croisy, Alain; Carrez, Daniele; Huel, Christiane; Chiaroni, Angele; Ducrot, Pierre; Bisagni, Emile; Jin, Lu; Leclercq, Guy
CORPORATE SOURCE: UMR 176 CNRS Institut Curie-Recherche, Laboratoire Raymond Latarjet, UMR 176 CNRS Institut Curie-Recherche, Laboratoire Raymond Latarjet, Centre Universitaire, Orsay, 91405, Fr.
SOURCE: Bioorganic & Medicinal Chemistry (2000), 8(11), 2629-2641
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:100750
GI



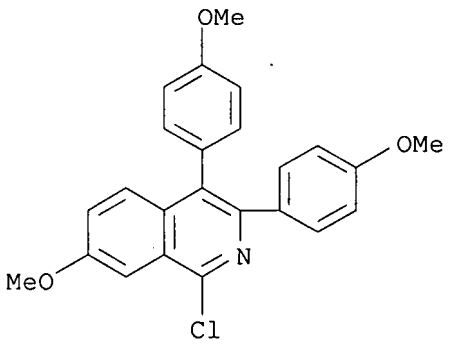
I

AB The synthesis of a series of 35 substituted 3,4-di-phenylquinolines and -isoquinolines is described. The majority of these mols. differ from all other triphenylethylene based antiestrogens by a different spatial location of the aminoalkyl side chain. The binding affinity of the most representative mols., including analogs without the side chain, for the estrogen receptor α (ER) was determined The ability of these mols. to induce the progesterone receptor was also studied. Antiproliferative activity was evaluated on MCF-7 human breast cancer cells, while intrinsic cytotoxic/cytostatic properties resulting from interaction with other targets than ER were assayed on L1210 murine leukemia cells. Introduction of an aminoalkylamino side chain at carbon 2 confers strong cytotoxic properties to diphenylquinolines as well as pure antiestrogenic activities. However, cytotoxicity is so high with respect to antiestrogenicity that the latter was clearly observable only in one case (I). The structure of I was determined by X-ray crystallog. Mol. modeling of its docking within the hormone-binding domain of the receptor was subsequently undertaken. According to these results, the design of mols. with the side chain bound to the ethylene part of the tri-phenylethylene skeleton might generate compds. of potential pharmacol. interest.

IT 320371-39-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cytotoxicity and antiestrogenic activity of diphenylquinolines and -isoquinolines)

RN 320371-39-9 HCAPLUS

CN Isoquinoline, 1-chloro-7-methoxy-3,4-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 8 OF 31 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:712977 HCAPLUS
DOCUMENT NUMBER: 133:281699

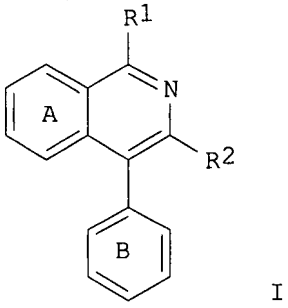
Updated Search

10572342

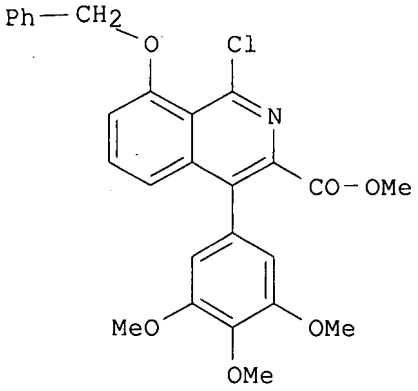
TITLE: Preparation of isoquinoline derivatives as phosphodiesterase V inhibitors
INVENTOR(S): Ukita, Shinzo; Yamada, Koichiro; Ohmori, Kenji; Yoshikawa, Kohei
PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 49 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000281654	A	20001010	JP 1999-83022	19990326
PRIORITY APPLN. INFO.:			JP 1999-83022	19990326

OTHER SOURCE(S): MARPAT 133:281699
GI



I



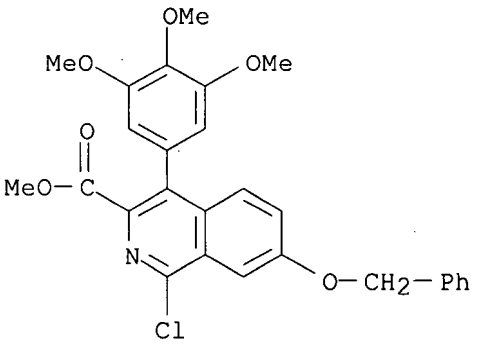
II

AB The title compds. I [ring A = benzene ring with substituents; ring B = (un)substituted benzene ring; R1 = (un)substituted alkoxy, halo, etc.; R2 = CO2R3, etc.; R3 = H, etc.], useful as phosphodiesterase V inhibitors (no data) for the treatment of circulatory system diseases (no data), are prepared For example, the title compound II was prepared

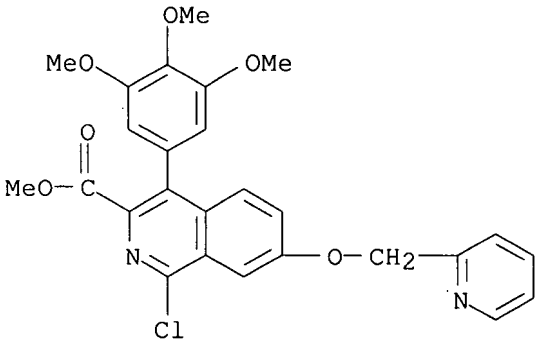
IT 299166-81-7P 299166-83-9P 299166-85-1P
299166-87-3P 299166-89-5P 299169-96-3P
299170-06-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of isoquinoline derivs. as phosphodiesterase V inhibitors)

RN 299166-81-7 HCAPLUS
CN 3-Isoquinolinecarboxylic acid, 1-chloro-7-(phenylmethoxy)-4-(3,4,5-trimethoxyphenyl)-, methyl ester (9CI) (CA INDEX NAME)

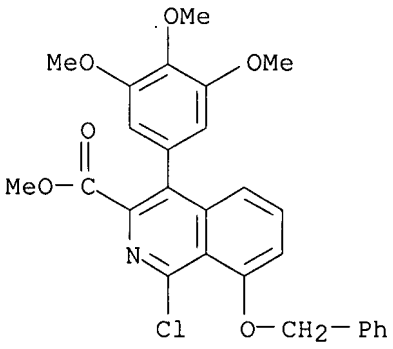
Updated Search



RN 299166-83-9 HCAPLUS
CN 3-Isoquinolinecarboxylic acid, 1-chloro-7-(2-pyridinylmethoxy)-4-(3,4,5-trimethoxyphenyl)-, methyl ester (9CI) (CA INDEX NAME)

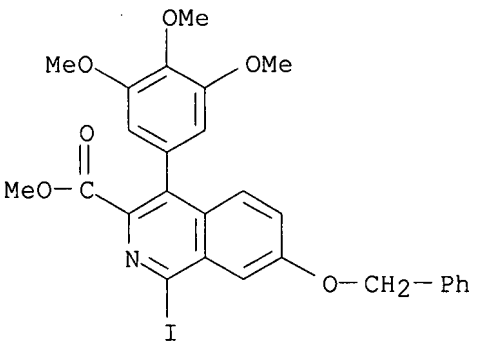


RN 299166-85-1 HCAPLUS
CN 3-Isoquinolinecarboxylic acid, 1-chloro-8-(phenylmethoxy)-4-(3,4,5-trimethoxyphenyl)-, methyl ester (9CI) (CA INDEX NAME)

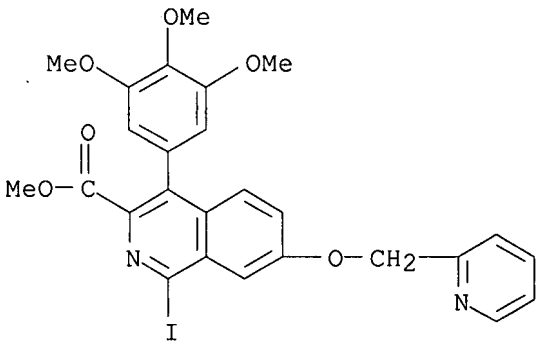


RN 299166-87-3 HCAPLUS
CN 3-Isoquinolinecarboxylic acid, 1-iodo-7-(phenylmethoxy)-4-(3,4,5-trimethoxyphenyl)-, methyl ester (9CI) (CA INDEX NAME)

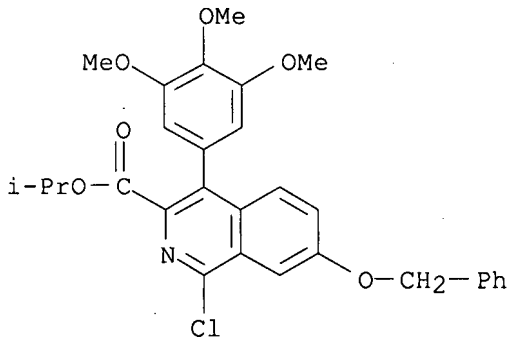
Updated Search



RN 299166-89-5 HCAPLUS
CN 3-Isoquinolinecarboxylic acid, 1-iodo-7-(2-pyridinylmethoxy)-4-(3,4,5-trimethoxyphenyl)-, methyl ester (9CI) (CA INDEX NAME)

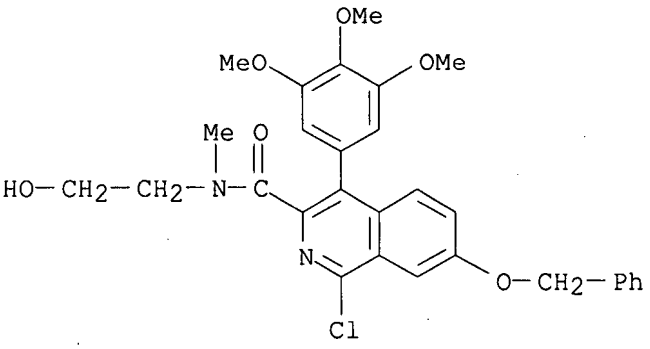


RN 299169-96-3 HCAPLUS
CN 3-Isoquinolinecarboxylic acid, 1-chloro-7-(phenylmethoxy)-4-(3,4,5-trimethoxyphenyl)-, 1-methylethyl ester (9CI) (CA INDEX NAME)

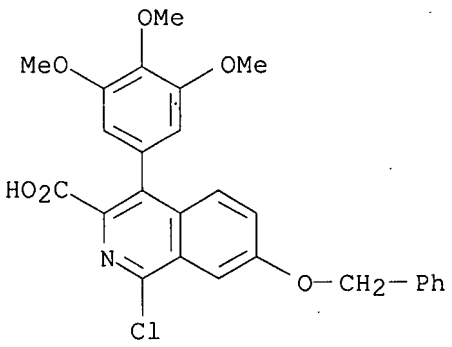


RN 299170-06-2 HCAPLUS
CN 3-Isoquinolinecarboxamide, 1-chloro-N-(2-hydroxyethyl)-N-methyl-7-(phenylmethoxy)-4-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

Updated Search



IT 299170-41-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of isoquinoline derivs. as phosphodiesterase V inhibitors)
RN 299170-41-5 HCAPLUS
CN 3-Isoquinolinecarboxylic acid, 1-chloro-7-(phenylmethoxy)-4-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

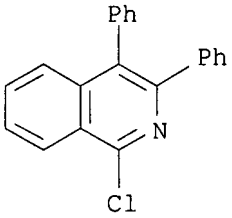


L14 ANSWER 9 OF 31 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:761240 HCAPLUS
DOCUMENT NUMBER: 123:339675
TITLE: Synthesis of 1-substituted 3,4-diarylisoquinoline derivatives
AUTHOR(S): Delcey, Martine Croisy; Huel, Christiane; Bisagni, Emile
CORPORATE SOURCE: Section de Biologie, Institut Curie, Orsay, 91405, Fr.
SOURCE: Heterocycles (1995), 41(8), 1721-30
CODEN: HTCYAM; ISSN: 0385-5414
PUBLISHER: Japan Institute of Heterocyclic Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 123:339675
AB 3,4-Diaryl-1(2H)-isoquinolinones and their 1-chloro derivs. were easily prepared by (1) condensation of 2-aroylbenzyl chlorides with arylmethylamines; (2) treatment of the resulting 1-aryl-1-hydroxy-N-(arylmethyl)isoindol-3-ones with LDA leading to an opening reaction and subsequent ring closure; (3) dehydration in boiling formic acid, which generally provided the expected isoquinolones in good yields; and (4) chlorination of the 2H-isoquinolin-1-ones by phosphorous oxychloride. In

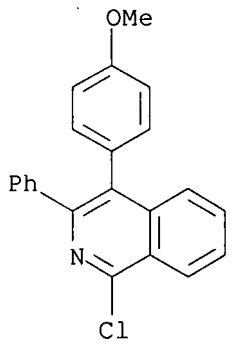
the cases of unsym. 4-hydroxy-3-(4-methoxyphenyl)-4-phenyl- and 4-hydroxy-4-(4-methoxyphenyl)-3-phenyl-1,2,3,4-tetrahydroisoquinolin-1-ones a partial migration and unexpected double aryl migrations (3→4) and (4→3) were observed

IT 102183-41-5P 170698-26-7P 170698-27-8P
170698-28-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

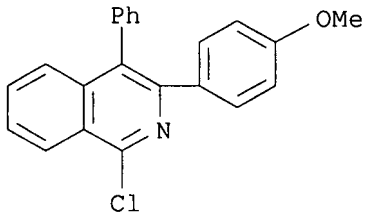
RN 102183-41-5 HCAPLUS
CN Isoquinoline, 1-chloro-3,4-diphenyl- (6CI, 9CI) (CA INDEX NAME)



RN 170698-26-7 HCAPLUS
CN Isoquinoline, 1-chloro-4-(4-methoxyphenyl)-3-phenyl- (9CI) (CA INDEX NAME)



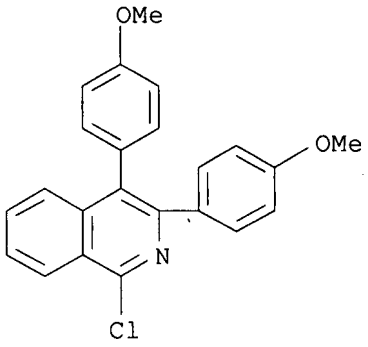
RN 170698-27-8 HCAPLUS
CN Isoquinoline, 1-chloro-3-(4-methoxyphenyl)-4-phenyl- (9CI) (CA INDEX NAME)



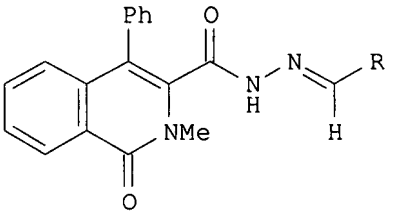
RN 170698-28-9 HCAPLUS
CN Isoquinoline, 1-chloro-3,4-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

Updated Search

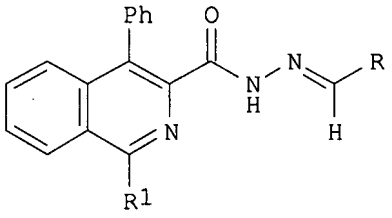
10572342



L14 ANSWER 10 OF 31 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:606104 HCAPLUS
DOCUMENT NUMBER: 123:83183
TITLE: Synthesis and antimicrobial evaluation of 4-phenyl-3-isoquinolinoyl-hydrazones
AUTHOR(S): Vittorio, Franco; Ronsisvalle, Giuseppe; Marrazzo, Agostino; Blandino, Giovanna
CORPORATE SOURCE: Inst. Chim. Farmaceutica e Tossicologica, Univ. Catania, Catania, 95125, Italy
SOURCE: Farmaco (1995), 50(4), 265-72
CODEN: FRMCE8
PUBLISHER: Societa Chimica Italiana
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



II

AB 2-Methyl-1-oxo-1,2-dihydro-3-carbazoyl-4-phenylisoquinoline, 1-methoxy- and 1-chloro-3-carbazoyl-4-phenylisoquinoline as well as a series of their 2-hydrazono-derivs. I (R = Ph, 4-O2NC6H4, 2-furyl, 2-naphthyl, etc.), II (R1 = OMe, Cl) were synthesized and evaluated for their antibacterial and antifungal activities, in vitro. I (R = 5-nitro-2-furyl) was fairly active against Staphylococcus aureus, Staphylococcus epidermidis, and streptococci group B.

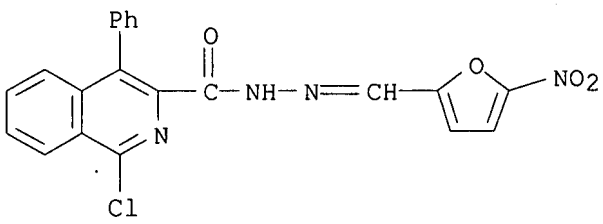
IT 164935-21-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis, bactericidal, and fungicidal activity of phenylisoquinolinoyl hydrazones)

RN 164935-21-1 HCAPLUS

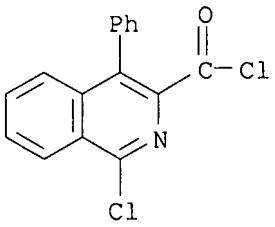
CN 3-Isoquinolinecarboxylic acid, 1-chloro-4-phenyl-, [(5-nitro-2-

Updated Search

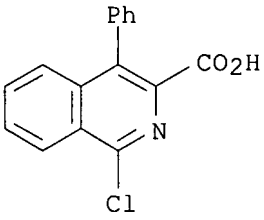
furanyl)methylene]hydrazide (9CI) (CA INDEX NAME)



IT 89928-71-2 89929-13-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis, bactericidal, and fungicidal activity of phenylisoquinolinoyl hydrazones)
RN 89928-71-2 HCAPLUS
CN 3-Isoquinolinecarbonyl chloride, 1-chloro-4-phenyl- (9CI) (CA INDEX NAME)

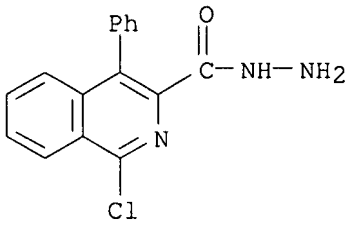


RN 89929-13-5 HCAPLUS
CN 3-Isoquinolinecarboxylic acid, 1-chloro-4-phenyl- (9CI) (CA INDEX NAME)

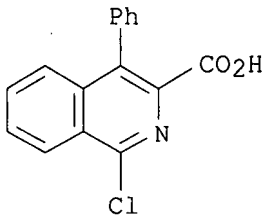


IT 164935-12-0P 164935-13-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis, bactericidal, and fungicidal activity of phenylisoquinolinoyl hydrazones)
RN 164935-12-0 HCAPLUS
CN 3-Isoquinolinecarboxylic acid, 1-chloro-4-phenyl-, hydrazide (9CI) (CA INDEX NAME)

Updated Search

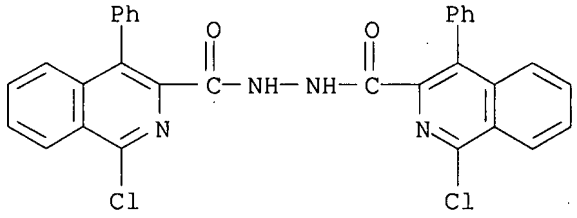


RN 164935-13-1 HCAPLUS
CN 3-Isoquinolinecarboxylic acid, 1-chloro-4-phenyl-, sodium salt (9CI) (CA INDEX NAME)

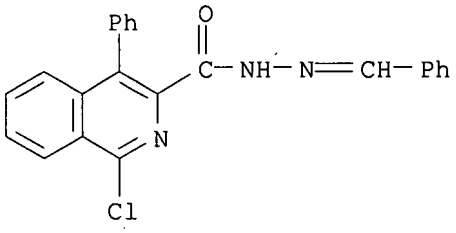


● Na

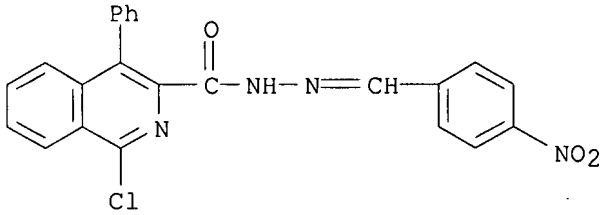
IT 164935-11-9P 164935-14-2P 164935-15-3P
164935-16-4P 164935-17-5P 164935-18-6P
164935-19-7P 164935-20-0P 164935-22-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis, bactericidal, and fungicidal activity of phenylisoquinolinoyl hydrazones)
RN 164935-11-9 HCAPLUS
CN 3-Isoquinolinecarboxylic acid, 1-chloro-4-phenyl-, 2-[(1-chloro-4-phenyl-3-isoquinolinyl)carbonyl]hydrazide (9CI) (CA INDEX NAME)



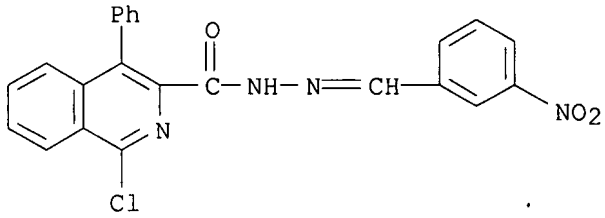
RN 164935-14-2 HCAPLUS
CN 3-Isoquinolinecarboxylic acid, 1-chloro-4-phenyl-, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)



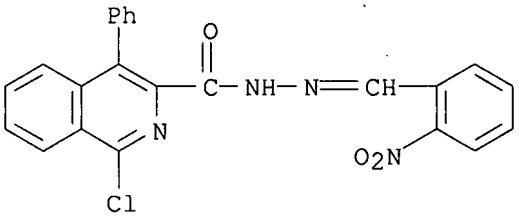
RN 164935-15-3 HCAPLUS
CN 3-Isoquinolinecarboxylic acid, 1-chloro-4-phenyl-, [(4-nitrophenyl)methylene]hydrazide (9CI) (CA INDEX NAME)



RN 164935-16-4 HCAPLUS
CN 3-Isoquinolinecarboxylic acid, 1-chloro-4-phenyl-, [(3-nitrophenyl)methylene]hydrazide (9CI) (CA INDEX NAME)

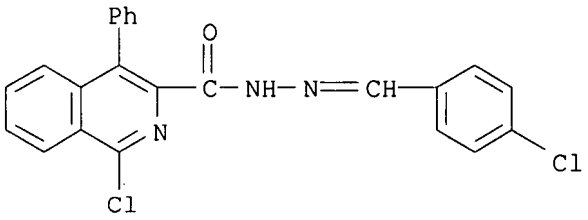


RN 164935-17-5 HCAPLUS
CN 3-Isoquinolinecarboxylic acid, 1-chloro-4-phenyl-, [(2-nitrophenyl)methylene]hydrazide (9CI) (CA INDEX NAME)

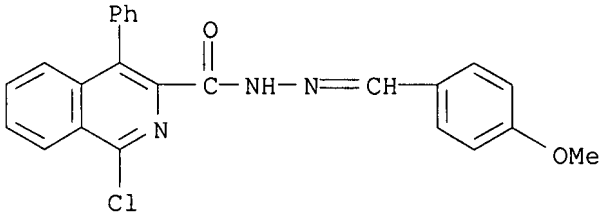


RN 164935-18-6 HCAPLUS
CN 3-Isoquinolinecarboxylic acid, 1-chloro-4-phenyl-, [(4-chlorophenyl)methylene]hydrazide (9CI) (CA INDEX NAME)

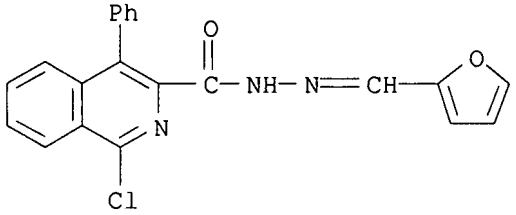
Updated Search



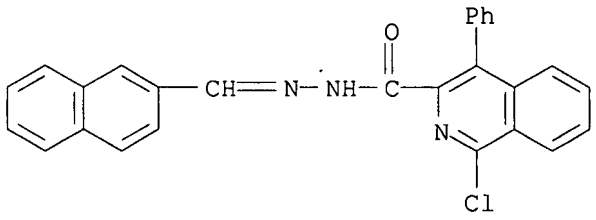
RN 164935-19-7 HCAPLUS
CN 3-Isoquinolinecarboxylic acid, 1-chloro-4-phenyl-, [(4-methoxyphenyl)methylene]hydrazide (9CI) (CA INDEX NAME)



RN 164935-20-0 HCAPLUS
CN 3-Isoquinolinecarboxylic acid, 1-chloro-4-phenyl-, (2-furanylmethylene)hydrazide (9CI) (CA INDEX NAME)



RN 164935-22-2 HCAPLUS
CN 3-Isoquinolinecarboxylic acid, 1-chloro-4-phenyl-, (2-naphthalenylmethylene)hydrazide (9CI) (CA INDEX NAME)



L14 ANSWER 11 OF 31 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:393124 HCAPLUS

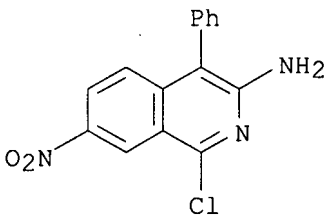
Updated Search

10572342

DOCUMENT NUMBER: 123:143784
TITLE: Transformations of polyfunctional 3-amino-1(2H)-isoquinolinones
AUTHOR(S): Volovenko, Yu. M.; Volovnenko, T. A.; Babichev, F. S.
CORPORATE SOURCE: Kiev. Univ., Kiev, Ukraine
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1994), (4), 515-20
CODEN: KGSSAQ; ISSN: 0132-6244
PUBLISHER: Latviiskii Institut Organicheskogo Sinteza
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I (R = CH2Ph, Me, CHMe2; R1 = CN) reacted with BzCl to give oxazinoisoquinolinones (II). I (R = CH2Ph, hexyl, Ph; R1 = CN) reacted with formamide to give pyrimidoisoquinolinones (III). Treatment of I (R = H, R1 = Ph) with POCl3/PCl5 gave chloroisoquinolinamine IV (R2 = Cl), which underwent substitution reactions to give IV (R2 = alkoxy, NHNH2, alkylamino, etc.). I (R = NH2, R1 = 1-methylbenzimidazol-2-yl) reacted with OC(COOEt)2 to give triazinoisoquinolinone V.
IT 166536-37-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and substitution reactions of)
RN 166536-37-4 HCAPLUS
CN 3-Isoquinolinamine, 1-chloro-7-nitro-4-phenyl- (9CI) (CA INDEX NAME)



L14 ANSWER 12 OF 31 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:257714 HCAPLUS
DOCUMENT NUMBER: 122:56051
TITLE: Condensed heterocyclic compounds, their production and use
INVENTOR(S): Natsugari, Hideaki; Ikeda, Hitoshi; Ishimaru, Takenori; Doi, Takayuki
PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan
SOURCE: Eur. Pat. Appl., 161 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

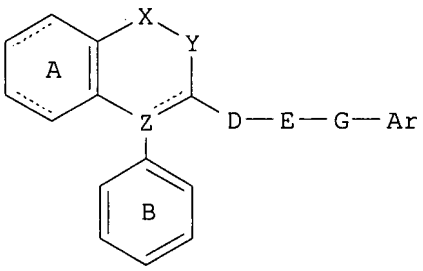
Updated Search

10572342

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 585913	A2	19940309	EP 1993-114024	19930902
EP 585913	A3	19940525		
EP 585913	B1	19971229		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
NO 9303133	A	19940307	NO 1993-3133	19930902
NO 179904	B	19960930		
NO 179904	C	19970108		
US 5482967	A	19960109	US 1993-114841	19930902
AT 161530	T	19980115	AT 1993-114024	19930902
CA 2105518	C	19940305	CA 1993-2105518	19930903
CA 2105518	A1	19940305		
AU 9346132	A	19940310	AU 1993-46132	19930903
AU 667739	B2	19960404		
FI 9303857	A	19940517	FI 1993-3857	19930903
JP 07010844	A	19950113	JP 1993-220333	19930903
JP 3724818	B2	20051207		
HU 67284	A2	19950328	HU 1993-2499	19930903
CN 1090274	A	19940803	CN 1993-118986	19930904
US 5700810	A	19971223	US 1995-540913	19951011
PRIORITY APPLN. INFO.:			JP 1992-237481 A	19920904
			JP 1993-103328 A	19930428
			US 1993-114841 A3	19930902

OTHER SOURCE(S): CASREACT 122:56051; MARPAT 122:56051

GI



I

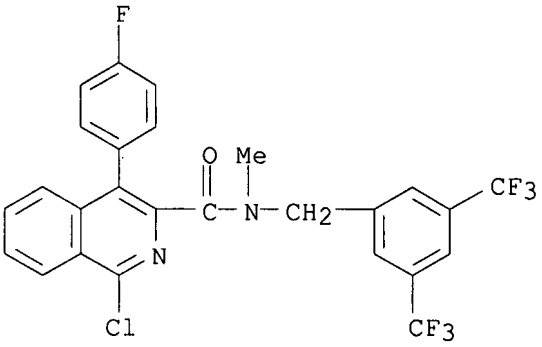
AB Novel compds. represented by I were prepared; ring A may be substituted; ring B represents an optionally substituted benzene ring; either X or Y represents -NR1- (R1 represents a hydrogen atom, an optionally substituted hydrocarbon group, an optionally substituted hydroxyl group or an optionally substituted amino group), -O- or -S-, the other representing -CO-, -CS-, or -C(R2)R2a- (R2 and R2a independently represent a hydrogen atom or an optionally substituted hydrocarbon group), or either X or Y represents -N=, the other representing =CR3- (R3 represents a hydrogen atom, a halogen atom, an optionally substituted hydrocarbon group, an optionally substituted amino group, a substituted hydroxyl group or a mercapto group substituted by an optionally substituted hydrocarbon group); ---- represents a single or double bond; when ---- is a single bond, Z represents -CR4- (R4 represents a hydrogen atom, hydroxyl group or an optionally substituted hydrocarbon group) or a nitrogen atom, or (ii) when ---- is a double bond, Z represents a carbon atom. D represents a C1-3 alkylene group which may be substituted by an oxo group or a thioxo

Updated Search

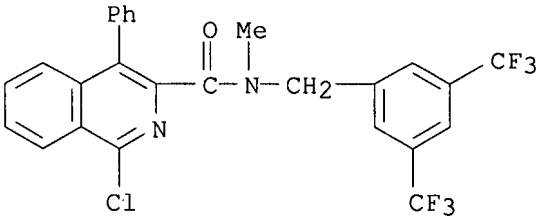
group, or D and Y, taken together, may form a 5- to 7-membered ring which may be substituted by an oxo group or a thioxo group; E represents -NR5- (R5 represents a hydrogen atom or an optionally substituted hydrocarbon group), -O- or -S-(O)n- (n is 0, 1 or 2), or R5 and Y, taken together, may form a 5- to 7-membered ring which may be substituted by an oxo group or a thioxo group. G represents a bond or a C1-3 alkylene group. Ar represents an optionally substituted aryl or heterocyclic group. Some representative prepared compds. were benzopyran-, quinoline-, isoquinoline- and quinoxalinecarboxamides. I and its salts have an excellent activity of inhibiting ACAT, lowering cholesterol in blood and inhibiting tachykinin receptor (test data given).

IT 159818-74-3P 159818-76-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and biol. activity of)

RN 159818-74-3 HCAPLUS
CN 3-Isoquinolinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-1-chloro-4-(4-fluorophenyl)-N-methyl- (9CI) (CA INDEX NAME)



RN 159818-76-5 HCAPLUS
CN 3-Isoquinolinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-1-chloro-N-methyl-4-phenyl- (9CI) (CA INDEX NAME)

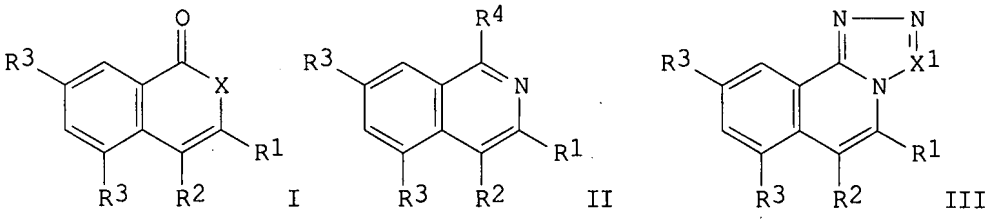


L14 ANSWER 13 OF 31 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1993:649888 HCAPLUS
DOCUMENT NUMBER: 119:249888
TITLE: Synthesis of some triazolo- and tetrazoloisoquinolines
AUTHOR(S): Bhide, B. H.; Akolkar, V. D.; Brahmbhatt, D. I.
CORPORATE SOURCE: Dep. Chem., Sardar Patel Univ., Vallabh Vidyanagar, 388 120, India
SOURCE: Indian Journal of Chemistry, Section B: Organic

Updated Search

10572342

Chemistry Including Medicinal Chemistry (1993), 32B(6), 675-8
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 119:249888
GI

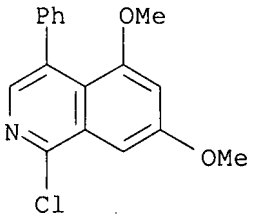


I II III

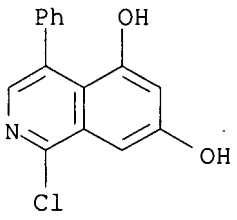
AB Treatment of isocoumarins I (X = O, R1 = H, Me, R2 = H, Ph, R3 = H, OH, OMe) with ammonia-ethanol gives isoquinolones I (X = NH), which react with POCl3-PCl5 affording 1-chloroisoquinolines II (R4 = Cl). Further reaction of II (R4 = Cl) with N2H4 furnishes 1-hydrazinoisoquinolines II (R4 = NHNH2), which on treatment with HCO2H and NaNO2/HCl provide triazoloisoquinolines III (X1 = CH) and tetrazoloisoquinolines III (X1 = N).

IT 151070-21-2P 151070-22-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and substitution of, with hydrazine)

RN 151070-21-2 HCAPLUS
CN Isoquinoline, 1-chloro-5,7-dimethoxy-4-phenyl- (9CI) (CA INDEX NAME)



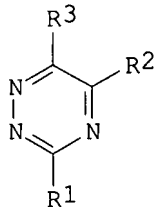
RN 151070-22-3 HCAPLUS
CN 5,7-Isoquinolinediol, 1-chloro-4-phenyl- (9CI) (CA INDEX NAME)



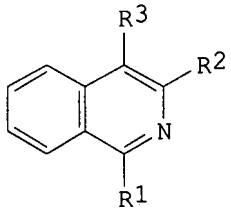
Updated Search

10572342

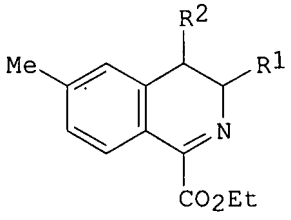
L14 ANSWER 14 OF 31 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1992:651216 HCAPLUS
DOCUMENT NUMBER: 117:251216
TITLE: Synthesis of isoquinolines by cycloaddition of arynes to 1,2,4-triazines
AUTHOR(S): Gonsalves, Antonio M. D. Rocha; Pinho e Melo, Teresa M. V. D.; Gilchrist, Thomas L.
CORPORATE SOURCE: Fac. Cienc. Tecnol., Univ. Coimbra, Port.
SOURCE: Tetrahedron (1992), 48(33), 6821-6
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 117:251216
GI



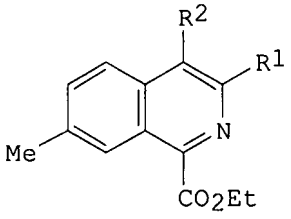
I



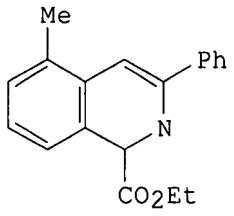
II



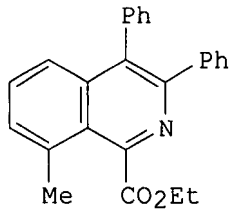
III



IV



V



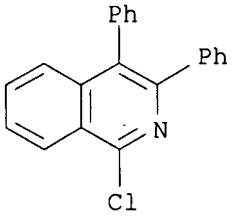
VI

AB Benzyne was generated from benzenediazonium-2-carboxylate in the presence of several 1,2,4-triazines I (R1 = Cl, Me, CO2Et; R2 = Ph, Me, H, CO2Et; R3 = Ph, Me, CO2Et) to give isoquinolines II in moderate yield. 1-Aminobenzotriazole was also used as a source of benzyne to again give isoquinolines in moderate yield. 4-Methylbenzyne, which was generated from 5-methylanthranilic acid, reacted unselectively with the triazines to give mixts. of 6- and 7-methylisoquinolines III and IV (R1 = Ph, R2 = H; R1 = R2 = Ph, CO2Et). On the other hand reactions of 3-methylbenzyne with the triazines I (R1 = CO2Et, R2 = H, Ph, R3 = Ph) proceeded with high regioselectivity, giving only the 5-methylisoquinoline V and the 8-methylisoquinoline VI, resp.

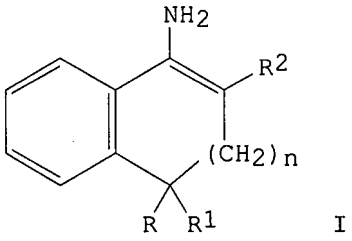
IT 102183-41-5P, 1-Chloro-3,4-diphenylisoquinoline
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 102183-41-5 HCAPLUS
CN Isoquinoline, 1-chloro-3,4-diphenyl- (6CI, 9CI) (CA INDEX NAME)

Updated Search

10572342



L14 ANSWER 15 OF 31 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1990:611797 HCAPLUS
DOCUMENT NUMBER: 113:211797
TITLE: Application of (2-cyanoaryl)arylacetonitriles in cyclization and annulation reactions. Preparation of 3-arylindans, 4-aryl-3,4-dihydronaphthalenes, 4-arylisoquinolines, 1-aminonaphthalenes, and heterocyclic analogues
AUTHOR(S): Sommer, Michael Bech; Begtrup, Mikael; Boegesoe, Klaus Peter
CORPORATE SOURCE: H. Lundbeck A/S, Copenhagen, DK-2500, Den.
SOURCE: Journal of Organic Chemistry (1990), 55(16), 4822-7
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 113:211797
GI



I

AB (2-Cyanoaryl)arylacetonitriles, obtained from o-halogen-substituted cyanoaroms. and arylacetonitriles, may be alkylated with Me chloroacetate. Subsequent abstraction of the proton adjacent to the ester group followed by attack of the anion at the aromatic cyano group gives rise to annulated 1-aminocyclopentenes, e.g., I (R = Ph, substituted Ph, R1 = cyano, R2 = CO2Me, n = o) by a Dieckmann-type reaction. The homologous esters similarly produce annulated 1-aminocyclohexenes I (n = 1). The generality of this annulation method is demonstrated by preparation of derivs. of 1-amino-1H-indene, 4-amino-6H-cyclopenta[b]thiophene, 5-amino-7H-pyridine, 1-amino-3,4-dihydronaphthalene, and 5-amino-2,9-dihydro-1H-cyclopent[c]isoquinoline. Hydrolysis and decarboxylation of these compds. leads to ketones as exemplified by synthesis of 3-arylindan-1-ones and 4-aryl-3,4-dihydro-1(2H)-naphthalen-1-ones. When treated with HBr, the (2-cyanophenyl)phenylacetonitriles cyclize to [3,4]-condensed 3-bromo-5-aryl-6-aminopyridines. Thus, derivs. of isoquinoline, thieno[3,2-c]pyridine, and 1,6-naphthyridine were prepared

IT 127999-80-8P

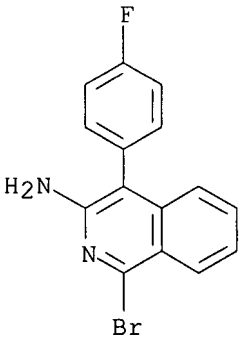
Updated Search

10572342

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and debromination of)

RN 127999-80-8 HCAPLUS

CN 3-Isoquinolinamine, 1-bromo-4-(4-fluorophenyl)- (9CI) (CA INDEX NAME)



L14 ANSWER 16 OF 31 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1984:185341 HCAPLUS

DOCUMENT NUMBER: 100:185341

TITLE: Studies on alkyl and aryl derivatives of isoquinoline. Part II. Synthesis and pharmacological activity of dialkylaminoalkyl esters of 1-chloro-3-carboxy-4-methylisoquinoline and corresponding 4-phenyl derivatives

AUTHOR(S): Vittorio, F.; Santagati, N. A.; Lancetta, T.; Duro, F.; Reina, R. Arrigo; Cosentino, C.

CORPORATE SOURCE: Ist. Chim. Farm. Tossicol., Univ. Catania, Catania, Italy

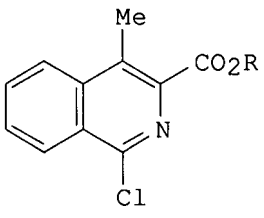
SOURCE: Farmaco, Edizione Scientifica (1984), 39(3), 217-28
CODEN: FRPSAX; ISSN: 0430-0920

DOCUMENT TYPE: Journal

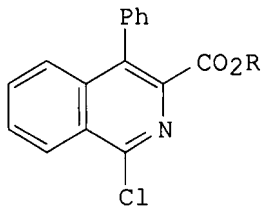
LANGUAGE: Italian

OTHER SOURCE(S): CASREACT 100:185341

GI



I



II

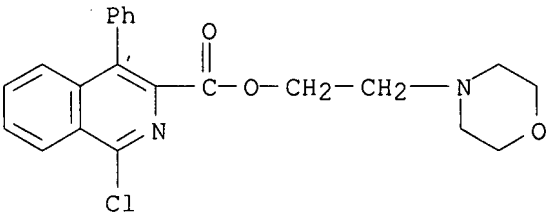
AB Six dialkylaminoalkyl 1-chloro-3-carboxy-4-methylisoquinolines (I; R = dialkylaminoalkyl) and 3 dialkylaminoethyl 1-chloro-3-carboxy-4-phenylisoquinolines (II; R = dialkylaminoethyl) were prepared from 3-carboxy-4-methylisocoumarinic acid [56661-74-6] and 1-chloro-3-carboxymethyl-4-phenylisoquinoline [56661-82-6], resp., and 6 of the 9 esters were screened pharmacol. I and II had antispasmodic activity; I were the less toxic. The compds. had no anticonvulsant or

Updated Search

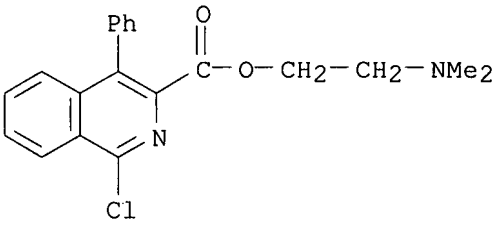
hypnotic activities. II, but not I, had slight analgesic and anti-inflammatory activities.

IT 89928-75-6 89928-76-7 89928-77-8
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pharmacol. of)

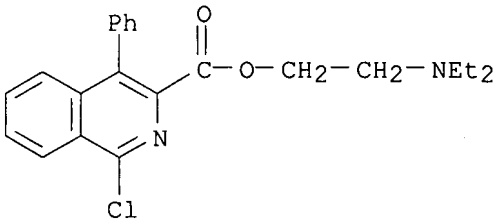
RN 89928-75-6 HCAPLUS
CN 3-Isoquinolinecarboxylic acid, 1-chloro-4-phenyl-, 2-(4-morpholinyl)ethyl ester (9CI) (CA INDEX NAME)



RN 89928-76-7 HCAPLUS
CN 3-Isoquinolinecarboxylic acid, 1-chloro-4-phenyl-, 2-(dimethylamino)ethyl ester (9CI) (CA INDEX NAME)



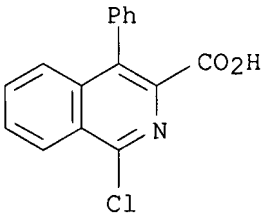
RN 89928-77-8 HCAPLUS
CN 3-Isoquinolinecarboxylic acid, 1-chloro-4-phenyl-, 2-(diethylamino)ethyl ester (9CI) (CA INDEX NAME)



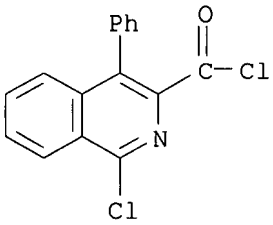
IT 89929-13-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and acid chlorination of)

RN 89929-13-5 HCAPLUS
CN 3-Isoquinolinecarboxylic acid, 1-chloro-4-phenyl- (9CI) (CA INDEX NAME)

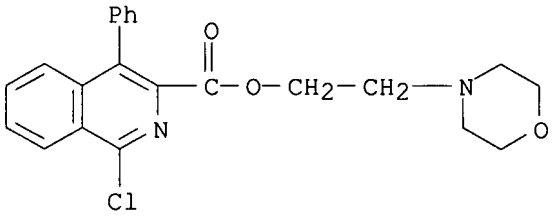
Updated Search



IT 89928-71-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and esterification of)
RN 89928-71-2 HCAPLUS
CN 3-Isoquinolinecarbonyl chloride, 1-chloro-4-phenyl- (9CI) (CA INDEX NAME)



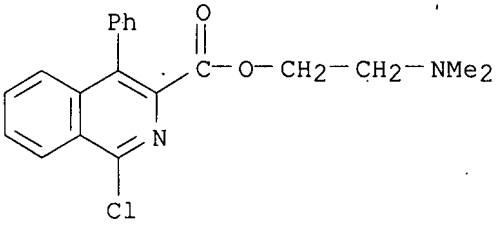
IT 89928-72-3P 89928-73-4P 89928-74-5P
89929-13-5DP, dialkylaminoalkyl esters
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(preparation and pharmacol. of)
RN 89928-72-3 HCAPLUS
CN 3-Isoquinolinecarboxylic acid, 1-chloro-4-phenyl-, 2-(4-morpholinyl)ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

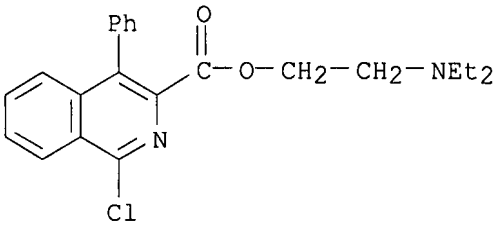
RN 89928-73-4 HCAPLUS
CN 3-Isoquinolinecarboxylic acid, 1-chloro-4-phenyl-, 2-(dimethylamino)ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Updated Search



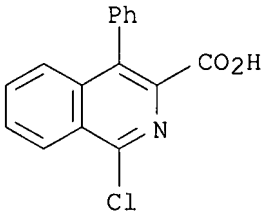
● HCl

RN 89928-74-5 HCAPLUS
CN 3-Isoquinolinecarboxylic acid, 1-chloro-4-phenyl-, 2-(diethylamino)ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 89929-13-5 HCAPLUS
CN 3-Isoquinolinecarboxylic acid, 1-chloro-4-phenyl- (9CI) (CA INDEX NAME)



IT 78945-98-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(saponification of)
RN 78945-98-9 HCAPLUS
CN 3-Isoquinolinecarboxylic acid, 1-chloro-4-phenyl-, methyl ester (9CI) (CA INDEX NAME)

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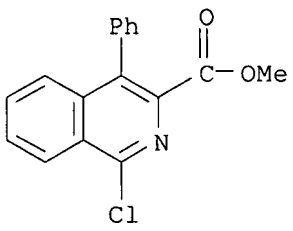
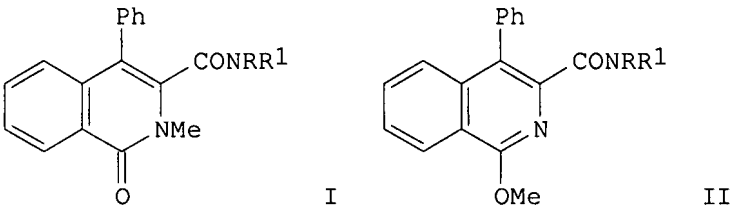


L14 ANSWER 17 OF 31 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1981:515239 HCAPLUS
DOCUMENT NUMBER: 95:115239
TITLE: Synthesis and pharmacological activity of amino- and dialkylaminoalkylamide derivatives of 3-carboxy-4-phenylisoquinoline. Part I
AUTHOR(S): Duro, F.; Santagati, N. A.; Vittorio, F.
CORPORATE SOURCE: Ist. Chim. Farm. Tossicol., Univ. Catania, Catania, Italy
SOURCE: Farmaco, Edizione Scientifica (1981), 36(6), 400-11
CODEN: FRPSAX; ISSN: 0430-0920
DOCUMENT TYPE: Journal
LANGUAGE: Italian
OTHER SOURCE(S): CASREACT 95:115239
GI



I II

AB 3-Isoquinolinecarboxamides I and II [R = H, R1 = ω-(dialkylaminoalkyl; NRR1 = morpholino, piperidino, pyrrolidino, 4-methyl-1-piperazinyl] were prepared and they exhibited spasmolytic, anesthetic, and antiinflammatory activity. 2-Methyl-4-phenyl-1,2-dihydro-2-oxo-3-isoquinolinecarbonyl chloride was treated with H2NCH2CH2NMe2 in C6H6 to give I (R = H, R1 = CH2CH2NMe2).
IT 78945-98-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and substitution reaction of, with sodium methoxide, saponification in)
RN 78945-98-9 HCAPLUS
CN 3-Isoquinolinecarboxylic acid, 1-chloro-4-phenyl-, methyl ester (9CI) (CA INDEX NAME)

Updated Search

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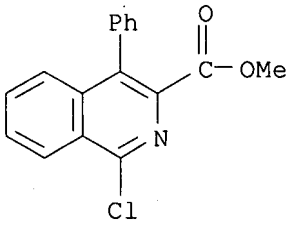
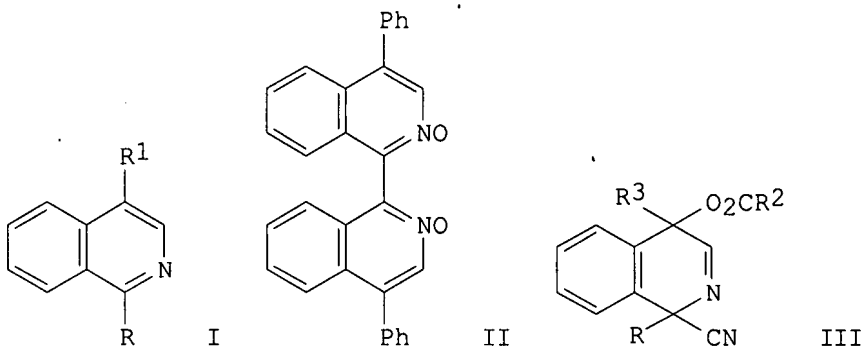


L14 ANSWER 18 OF 31 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1978:120952 HCAPLUS
DOCUMENT NUMBER: 88:120952
TITLE: The reaction of heteroaromatic N-oxides with acid chloride and cyanide. V. On the reaction of 1-substituted and 1,4-disubstituted isoquinoline 2-oxides with aroyl chloride and potassium cyanide
AUTHOR(S): Hayashi, Eisaku; Miyashita, Akira
CORPORATE SOURCE: Shizuoka Coll. Pharm., Shizuoka, Japan
SOURCE: Yakugaku Zasshi (1977), 97(12), 1334-44
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
OTHER SOURCE(S): CASREACT 88:120952
GI



AB Nine isoquinolines or their N-oxides I (R = Ph, CN, CH2Ph, Me, Et, Bu; R1 = H) and the diisoquinolinyl dioxide II were treated with R2COCl (R2 = Ph, 2-furyl, p-MeOC6H4, 3-pyridyl, p-NO2C6H4) and KCN to give I (R1 = O2CR2) and the dihydro derivs. III (R3 = H), whereas the N-oxides of disubstituted isoquinolines (I, R = Ph, Et, CN; R1 = Ph) gave only III (R3 = Ph).

IT 65810-96-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)

RN 65810-96-0 HCAPLUS

CN Isoquinoline, 1-chloro-4-phenyl- (6CI, 9CI) (CA INDEX NAME)

Updated Search

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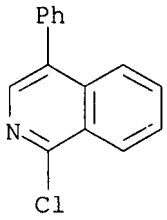
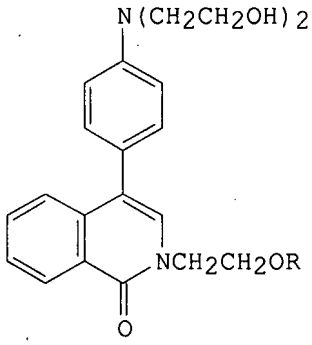
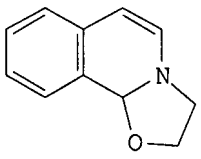


L14 ANSWER 19 OF 31 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1978:89492 HCAPLUS
DOCUMENT NUMBER: 88:89492
TITLE: Isoquinolines. 7. Reaction of ethylene oxide with isoquinolines. Novel isoquinolone and oxazolidine formation
AUTHOR(S): Filer, Crist N.; Granchelli, Felix E.; Soloway, Albert H.; Neumeyer, John L.
CORPORATE SOURCE: Coll. Pharm. Allied Health Prof., Northeast. Univ., Boston, MA, USA
SOURCE: Journal of Organic Chemistry (1978), 43(4), 672-5
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 88:89492
GI



III



IV

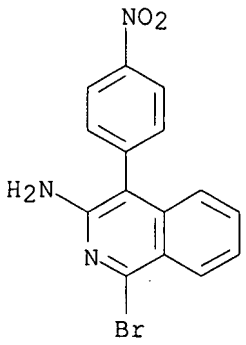
AB Aprotic deamination of 3-amino-1-bromo-4-(4-nitrophenyl)isoquinoline followed by partial reduction yielded 4-(4-aminophenyl)-1-bromoisoquinoline (I), and complete reduction yielded 4-(4-aminophenyl)isoquinoline (II). Isoquinolines I and II, when treated with excess ethylene oxide in AcOH gave the isoquinolones III (R = H, Ac). The mechanism involved an oxazolidine intermediate. When isoquinoline was similarly treated with ethylene oxide, 2,3-dihydro-10bH-oxazolo[2,3-a]isoquinoline (IV) was obtained.

IT 31309-65-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(deamination of)

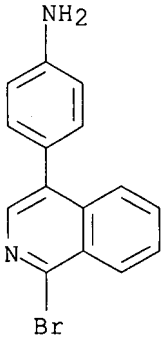
RN 31309-65-6 HCAPLUS
CN 3-Isoquinolinamine, 1-bromo-4-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

Updated Search

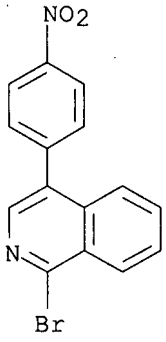
10572342



IT 64345-80-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with ethylene oxide)
RN 64345-80-8 HCAPLUS
CN Benzenamine, 4-(1-bromo-4-isoquinolinyl)- (9CI) (CA INDEX NAME)



IT 64345-81-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
RN 64345-81-9 HCAPLUS
CN Isoquinoline, 1-bromo-4-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

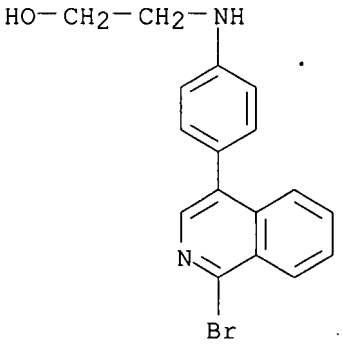


IT 64345-76-2P 64345-78-4P

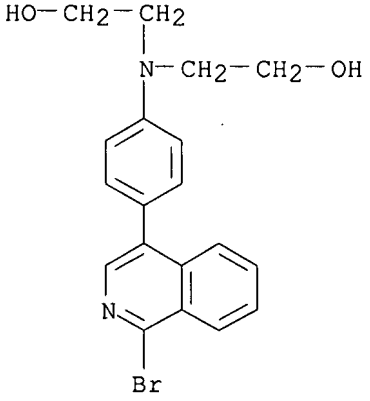
Updated Search

10572342

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 64345-76-2 HCAPLUS
CN Ethanol, 2-[[4-(1-bromo-4-isoquinolinyl)phenyl]amino]- (9CI) (CA INDEX NAME)

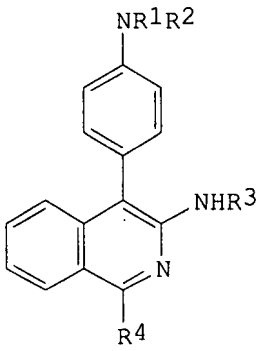


RN 64345-78-4 HCAPLUS
CN Ethanol, 2,2'-[[4-(1-bromo-4-isoquinolinyl)phenyl]imino]bis- (9CI) (CA INDEX NAME)



L14 ANSWER 20 OF 31 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1977:561588 HCAPLUS
DOCUMENT NUMBER: 87:161588
TITLE: Isoquinolines. 6. Potential central nervous system antitumor agents. Nitrogen mustards of 3-amino-4-(p-aminophenyl)isoquinoline
AUTHOR(S): Filer, Crist N.; Granchelli, Felix E.; Soloway, Albert H.; Neumeyer, John L.
CORPORATE SOURCE: Coll. Pharm. Allied Health Prof., Northeast. Univ., Boston, MA, USA
SOURCE: Journal of Medicinal Chemistry (1977), 20(11), 1504-8
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 87:161588
GI

Updated Search



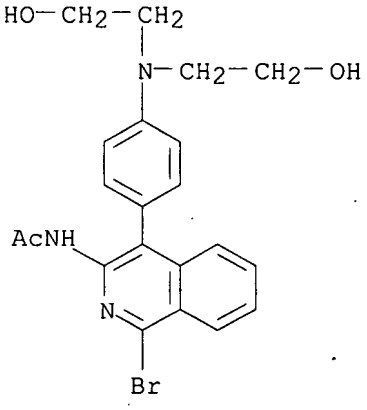
I

AB Six title compds. (I:R1 = H, CH2CH2Cl; R2 = CH2CH2Cl, COCH2N(CH2CH2Cl)2, COCH2CH2N(CH2CH2Cl)2, CH2CH2N(CH2CH2Cl)2; R3 = Ac, H, Et; R4 = H, Br) were prepared from the appropriate diol precursors using SOCl2. Most of the intermediates and all title compds. were tested in the i.p. murine leukemia L1210 system, but none were active.

IT 64157-36-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and chlorination of)

RN 64157-36-4 HCAPLUS

CN Acetamide, N-[4-[4-[bis(2-hydroxyethyl)amino]phenyl]-1-bromo-3-isoquinolinyl]- (9CI) (CA INDEX NAME)



IT 64157-44-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as neoplasm inhibitor)

RN 64157-44-4 HCAPLUS

CN Acetamide, N-[4-[4-[bis(2-chloroethyl)amino]phenyl]-1-bromo-3-isoquinolinyl]-, monohydrochloride (9CI) (CA INDEX NAME)

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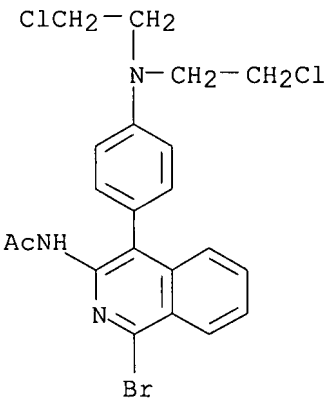
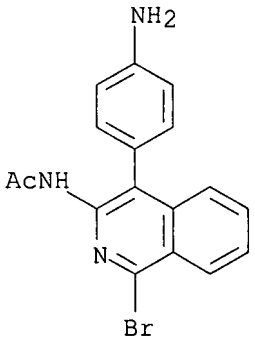


● HCl

IT 64157-54-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with ethylene oxide)
RN 64157-54-6 HCAPLUS
CN Acetamide, N-[4-(4-aminophenyl)-1-bromo-3-isoquinolinyl]- (9CI) (CA INDEX NAME)



L14 ANSWER 21 OF 31 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1977:89634 HCAPLUS
DOCUMENT NUMBER: 86:89634
TITLE: 3-Substituted 4-aryl isoquinolines
INVENTOR(S): Houlihan, William J.; Nadelson, Jeffrey
PATENT ASSIGNEE(S): Sandoz-Wander, Inc., USA
SOURCE: U.S., 8 pp. Division of U.S. 3,872,125.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

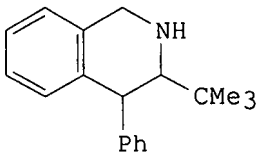
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3989704	A	19761102	US 1975-542843	19750121

Updated Search

10572342

US 3872125	A	19750318	US 1973-411074		19731030
US 4175191	A	19791120	US 1977-852503		19771117
PRIORITY APPLN. INFO.:			US 1972-259860	A2	19720605
			US 1973-339616	A2	19730303
			US 1973-411074	A3	19731030
			US 1975-542843	A3	19750121
			US 1976-705703	A1	19760715

GI



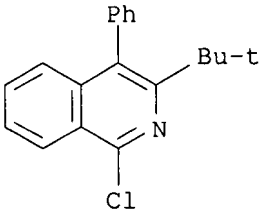
II

AB Hydrogenation of 3-tert-butyl-4-phenylisoquinoline (I) in AcOH over PtO2 at 20°/50 psi gives II, effective as antidiabetic. I is obtained by reaction of PhCONHMe with PhCHO to give 2-[PhCH(OH)]C6H4CONHMe which is cyclized to 3-phenylphthalide (III). Hydrogenation of III gives 2-(PhCH2)C6H4CO2H which is converted with Me3CNH2 to 2-(PhCH2)C6H4CONHCMe3 (IV). Reaction of IV with Me3CCOCl gives 2-[PhCH(COCMe3)]C6H4CONHCMe3 which on treatment with polyphosphoric acid gives 3-tert-butyl-4-phenylisocarbostyril which is converted to I via 3-tert-butyl-1-chloro-4-phenylisoquinoline.

IT 55792-01-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and dechlorination of)

RN 55792-01-3 HCAPLUS

CN Isoquinoline, 1-chloro-3-(1,1-dimethylethyl)-4-phenyl- (9CI) (CA INDEX NAME)



L14 ANSWER 22 OF 31 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:	1975:428123 HCAPLUS
DOCUMENT NUMBER:	83:28123
TITLE:	3-Substituted-4-aryl isoquinolines
INVENTOR(S):	Houlihan, William J.; Nadelson, Jeffrey
PATENT ASSIGNEE(S):	Sandoz-Wander, Inc., USA
SOURCE:	U.S., 8 pp. CODEN: USXXAM
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	2

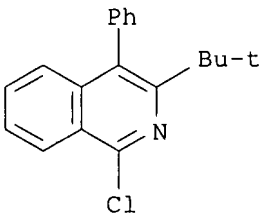
Updated Search

10572342

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3872125	A	19750318	US 1973-411074	19731030
US 3989704	A	19761102	US 1975-542843	19750121
US 4175191	A	19791120	US 1977-852503	19771117
PRIORITY APPLN. INFO.:			US 1972-259860	A2 19720605
			US 1973-339616	A2 19730303
			US 1973-411074	A3 19731030
			US 1975-542843	A3 19750121
			US 1976-705703	A1 19760715

OTHER SOURCE(S): MARPAT 83:28123
GI For diagram(s), see printed CA Issue.
AB Tetrahydroisoquinoline I, useful as an antidiabetic when administered orally at 100 mg twice a day, was prepared from lithiated PhCONHMe and BzH via o-PhCH(OH)C6H4CONHMe, 3-phenylphthalide, o-PhCH2C6H4CO2H, o-PhCH2C6H4CONHCMe3, o-PhCH(COCMe3)C6H4CONHCMe3, isocarbostyril II(R = OH), chloroisoquinoline II(R = Cl), and isoquinoline II(R = H)·HCl.
IT 55792-01-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and dechlorination of)
RN 55792-01-3 HCAPLUS
CN Isoquinoline, 1-chloro-3-(1,1-dimethylethyl)-4-phenyl- (9CI) (CA INDEX NAME)



L14 ANSWER 23 OF 31 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1975:409819 HCAPLUS
DOCUMENT NUMBER: 83:9819
TITLE: 2-Methyl-3-substituted-4-aryl isoquinolines
INVENTOR(S): Houlihan, William J.; Nadelson, Jeffrey
PATENT ASSIGNEE(S): Sandoz-Wander, Inc., USA
SOURCE: U.S., 8 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3870722	A	19750311	US 1973-412132	19731102
PRIORITY APPLN. INFO.:			US 1973-412132	A 19731102

GI For diagram(s), see printed CA Issue.
AB Four hypocholesterlemic (no data) isoquinolines I (R1 = tert-Bu, R2 = H, Me, MeO; R1 = 1-methylcyclohexyl, R2 = H) were prepared by HCO2H-HCHO

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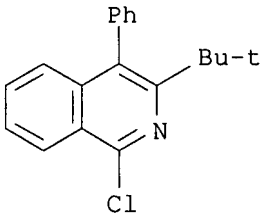
methylation of II. II(R1 = tert-Bu, R2 = H) was prepared from BzNHMe and BzH via o-HOCHPhC6H4CONHMe, phthalide III, o-PhCH2C6H4CO2H, o-PhCH2C6H4COCl,. o-PhCH2C6H4CONHCMe3, o-PhCH(COCMe3)C6H4CONHCMe3, isocarbostyryl IV, chloroisoquinoline V, and isoquinoline VI.

IT 55792-01-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrogenolysis of)

RN 55792-01-3 HCAPLUS

CN Isoquinoline, 1-chloro-3-(1,1-dimethylethyl)-4-phenyl- (9CI) (CA INDEX NAME)



L14 ANSWER 24 OF 31 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1975:16836 HCAPLUS
DOCUMENT NUMBER: 82:16836
TITLE: Hypolipemic and hypoglycemic 1-(1-imidazolyl)isoquinolines
INVENTOR(S): Lerch, Ulrich; Granzer, Ernold
PATENT ASSIGNEE(S): Farbwerke Hoechst A.-G.
SOURCE: Ger. Offen., 34 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2314985	A1	19741017	DE 1973-2314985	19730326
ES 424436	A1	19761101	ES 1974-424436	19740320
GB 1464289	A	19770209	GB 1974-12861	19740322
ZA 7401917	A	19750326	ZA 1974-1917	19740325
DD 114607	A5	19750812	DD 1974-177438	19740325
AU 7467098	A	19750925	AU 1974-67098	19740325
US 3914236	A	19751021	US 1974-454713	19740325
HU 168524	B	19760528	HU 1974-HO1659	19740325
AT 7402452	A	19761015	AT 1974-2452	19740325
AT 337183	B	19770610		
BE 812841	A1	19740926	BE 1974-142458	19740326
FR 2223024	A1	19741025	FR 1974-10396	19740326
JP 49126684	A	19741204	JP 1974-33183	19740326
US 3961062	A	19760601	US 1975-562048	19750326

PRIORITY APPLN. INFO.:
DE 1973-2314985 A 19730326
DE 1973-7314985 A 19730326
US 1974-454713 A3 19740325

GI For diagram(s), see printed CA Issue.

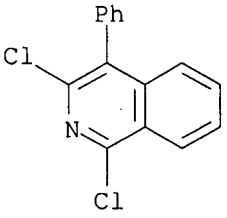
AB Nineteen imidazolyl-isoquinolines I (R = H, Cl, Ph, or Et; R1 = H, Ph,

cyclohexyl, Et, Bu, or Cl; R2, R3, R4 = H, Ph, or Me) and (or) their salts, e.g. hydrochlorides, were prepared by reaction of the corresponding 1-chloroisoquinolines with the imidazoles in the presence of NaH or KOH or Bu3N in, e.g., (MeOCH2)2 or DMF. I had hypolipemic and hypoglycemic activities in rats and rabbits.

IT 55150-48-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with imidazoles)

RN 55150-48-6 HCAPLUS

CN Isoquinoline, 1,3-dichloro-4-phenyl- (9CI) (CA INDEX NAME)



L14 ANSWER 25 OF 31 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1973:532897 HCAPLUS

DOCUMENT NUMBER: 79:132897

TITLE: Isoquinolines. 3. 3-Aminoisoquinoline derivatives with central nervous system depressant activity

AUTHOR(S): Neumeyer, John L.; Weinhardt, Klaus K.; Carrano, Richard A.; McCurdy, David H.

CORPORATE SOURCE: Arthur D. Little, Inc., Cambridge, MA, USA

SOURCE: Journal of Medicinal Chemistry (1973), 16(7), 808-13
CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

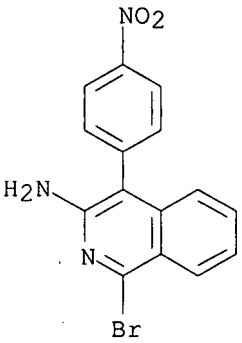
LANGUAGE: English

AB 3-Amino-4-(p-aminophenyl)isoquinoline (I) [31309-67-8] and 4-(p-acetamidophenyl)-3-aminoisoquinoline (II) [31309-69-0] showed central nervous depressant and anticonvulsant activity in mice. I and II depressed forced motor activity with ED50 values of 37.8 and 63.3 mg/kg i.p., resp., and were thus similar to phenobarbital and diphenylhydantoin in potency. Both compds. protected against electroshock convulsions and oxotremorine-induced tremor. To synthesize I, α-cyano-o-tolunitrile [3759-28-2] was reacted with p-nitrobromobenzene [586-78-7] under basic conditions to form α-cyano-α-(p-nitrophenyl)-o-tolunitrile [31309-64-5], which was cyclized with HBr to 3-amino-1-bromo-4-(p-nitrophenyl)isoquinoline [31309-65-6] and hydrogenated over Pd/C to I. I was acetylated with Ac2O in pyridine to II.

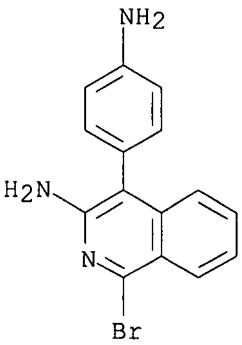
IT 31309-65-6P 31309-66-7P 49710-63-6P
49710-64-7P 49710-68-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 31309-65-6 HCAPLUS

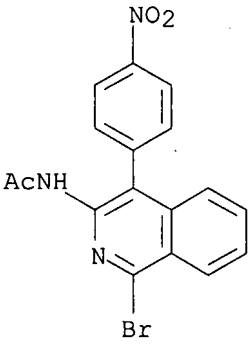
CN 3-Isoquinolinamine, 1-bromo-4-(4-nitrophenyl)- (9CI) (CA INDEX NAME)



RN 31309-66-7 HCAPLUS
CN 3-Isoquinolinamine, 4-(4-aminophenyl)-1-bromo- (9CI) (CA INDEX NAME)



RN 49710-63-6 HCAPLUS
CN Acetamide, N-[1-bromo-4-(4-nitrophenyl)-3-isoquinolinyl]- (9CI) (CA INDEX NAME)



RN 49710-64-7 HCAPLUS
CN Acetamide, N-acetyl-N-[1-bromo-4-(4-nitrophenyl)-3-isoquinolinyl]- (9CI) (CA INDEX NAME)

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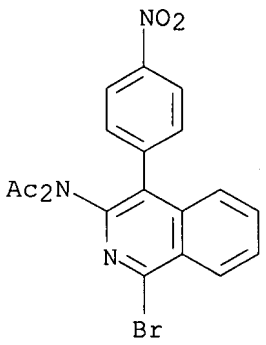
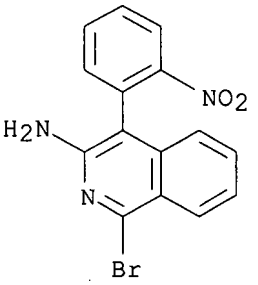


RN 49710-68-1 HCAPLUS
CN 3-Isoquinolinamine, 1-bromo-4-(2-nitrophenyl)- (9CI) (CA INDEX NAME)



L14 ANSWER 26 OF 31 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1971:99899 HCAPLUS
DOCUMENT NUMBER: 74:99899
TITLE: Central nervous system depressant 3-amino-4-(p-aminophenyl)isoquinoline derivatives
INVENTOR(S): Neumeyer, John L.; Weinhardt, Klaus K.
PATENT ASSIGNEE(S): Little, Arthur D., Inc.
SOURCE: Ger. Offen., 23 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2030675	A	19710211	DE 1970-2030675	19700622
PRIORITY APPLN. INFO.:			US 1969-835734 A	19690623

GI For diagram(s), see printed CA Issue.
AB The title compds. (I) and their pharmaceutically compatible salts were prepared by cyclization of p-O2NC6H4CH(CN)C6H4CN-o, obtained from p-BrC6H4NO2 and o-NCC6H4CH2CN, with HBr-KHCO3, and one- or two-step NO2 reduction and debromination. Acetylation of the formed I (R = R1 = H) gave I (R = H, R1 = Ac), and its B2H6 reduction I (R = H, R1 = Et).
IT 31309-65-6P 31309-66-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 31309-65-6 HCAPLUS

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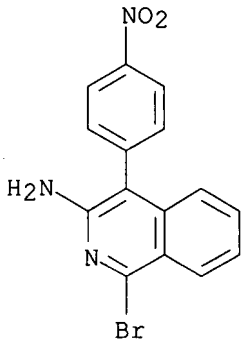
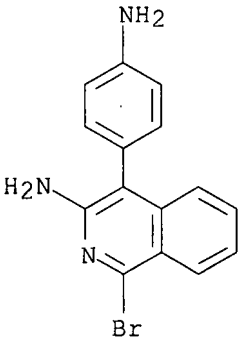
CN 3-Isoquinolinamine, 1-bromo-4-(4-nitrophenyl)- (9CI) (CA INDEX NAME)



RN 31309-66-7 HCAPLUS
CN 3-Isoquinolinamine, 4-(4-aminophenyl)-1-bromo- (9CI) (CA INDEX NAME)



L14 ANSWER 27 OF 31 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1960:78652 HCAPLUS
DOCUMENT NUMBER: 54:78652
ORIGINAL REFERENCE NO.: 54:14934f-h
TITLE: Ultraviolet spectra of some derivatives of 3- and 4-phenylisoquinoline
AUTHOR(S): Berti, Giancarlo; Corti, Piero
CORPORATE SOURCE: Univ. Pisa, Italy
SOURCE: Annali di Chimica (Rome, Italy) (1959), 49, 2110-23
CODEN: ANCRAI; ISSN: 0003-4592
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB The ultraviolet spectra in EtOH solution of the following substituted isoquinolines have been determined: 4-phenyl-, 3-methyl-4-phenyl-, 3-ethyl-4-phenyl-, 3-phenyl-, 3,4-diphenylisoquinoline, and their hydrochlorides; 1-chloro-4-phenyl-, 1-chloro-3-methyl-4-phenyl-, 1-chloro-3-ethyl-4-phenyl-, 1-chloro-3-phenyl-, 1-chloro-3,4-diphenylisoquinoline; 4-phenyl-, 2-methyl-4-phenyl-, 3-methyl-4-phenyl-, 3-ethyl-4-phenyl-, 3-phenyl-, 3,4-diphenylisocarbostyril. A phenyl group in the 4 position does not change much the characteristic isoquinoline spectrum, with 3 bands around 220, 280, and 320 mμ, while 3-phenylisoquinolines have quite different spectra, with bands around 250, 290, and 330 mμ; this shows much less fine structure. The

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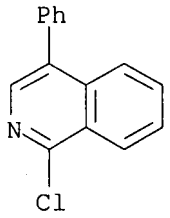
isoquinolinium salts are characterized by a strong band around 345 mμ. Absorption curves and tables of λmaximum and log ε for all the above compds. are included.

IT 65810-96-0, Isoquinoline, 1-chloro-4-phenyl-
(spectra of)

RN 65810-96-0 HCAPLUS

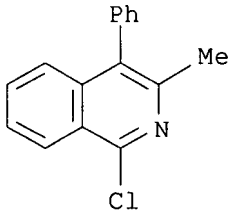
CN Isoquinoline, 1-chloro-4-phenyl- (6CI, 9CI) (CA INDEX NAME)



IT 101423-02-3, Isoquinoline, 1-chloro-3-methyl-4-phenyl-
101602-30-6, Isoquinoline, 1-chloro-3-ethyl-4-phenyl-
102183-41-5, Isoquinoline, 1-chloro-3,4-diphenyl-
(spectrum of)

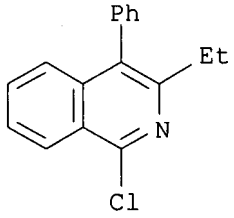
RN 101423-02-3 HCAPLUS

CN Isoquinoline, 1-chloro-3-methyl-4-phenyl- (6CI) (CA INDEX NAME)



RN 101602-30-6 HCAPLUS

CN Isoquinoline, 1-chloro-3-ethyl-4-phenyl- (6CI) (CA INDEX NAME)



RN 102183-41-5 HCAPLUS

CN Isoquinoline, 1-chloro-3,4-diphenyl- (6CI, 9CI) (CA INDEX NAME)

Updated Search

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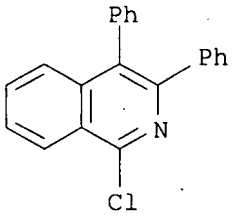

L14 ANSWER 28 OF 31 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1959:111808 HCAPLUS
DOCUMENT NUMBER: 53:111808
ORIGINAL REFERENCE NO.: 53:20063a-i,20064a
TITLE: Synthesis of isoquinoline derivatives
AUTHOR(S): Berti, Giancarlo; Corti, Piero
CORPORATE SOURCE: Univ. Pisa
SOURCE: Gazzetta Chimica Italiana (1958), 88, 704-13
CODEN: GCITA9; ISSN: 0016-5603
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 53:111808
GI For diagram(s), see printed CA Issue.
AB cf. C.A. 47, 4341i. Cyclization of the amides 2- RHNCOC6H4CPh:CR':Cl (I) gave the isocarbostyrils, C6H4.CO.NR.CR'CPh (II), readily converted to the corresponding 4-phenyl-3-substituted-isoquinolines (III). Cyclization of 2-ClCOC6H4CPh:CPhCl (IV) with PCl5 gave 2,3-dichloro-2,3-diphenyl-1-indanone (V). SOCl2 (2 g.) and 1 g. 2-HO2CC6H4CPh:CEtCl (VI) refluxed, the solution evaporated in vacuo, the residue taken up in C6H6, the solution saturated 10 min. with dry NH3, and the washed (H2O, dilute aqueous Na2CO3) and dried (MgSO4) solution concentrated and diluted with C6H6 gave 0.78 g. I (R = H, R' = Et) (VII), m. 124-5° (C6H6-ligroine). VII (0.7 g.) in 20 ml. 10% KOH in (CH2OH)2 refluxed 75 min. and the cooled solution diluted with H2O gave 0.52 g. II (R = H, R' = Et) (VIII), m. 255-7°. Titration of the aqueous filtrate according to Volhard showed 92% transformation to ionic Cl. VIII (0.45 g.) and 1 g. POCl3 heated 20 min. on a steam bath, the cooled solution poured onto ice, made alkaline with NaOH, the product extracted with boiling C6H6, the filtered extract evaporated to dryness, and the residue recrystd. (dilute MeOH) gave 0.37 g. 1-chloro-3-ethyl-4-phenylisoquinoline, m. 69-70°, which, hydrogenated (0.25 g.) 30 min. in 20 ml. alc. with 0.5 g. Pd-CaCO3 in 5 ml. 10% alc. KOH, the solution saturated with CO2, filtered, evaporated to dryness and the residue crystallized (dilute alc.) gave 0.14 g. III (3-substituent = Et), m. 64-6°. VI (1 g.) and 1 g. PCl5 heated to a homogeneous mass on a steam bath, taken up in C6H6, the solution washed rapidly with aqueous Na2CO3, treated with 1 g. PhNH2, the mixture boiled 10 min., the washed (HCl, H2O, aqueous Na2CO3) and dried (MgSO4) solution concentrated, and the concentrate diluted with C6H6 and filtered gave 0.65 g. I (R = Ph, R' = Et), cyclized (0.2 g.) by refluxing 90 min. with 5 ml. 10% KOH in (CH2OH)2 to II (R = Ph, R' = Et), m. 187-9° (C6H6-ligroine),with 98.5 % conversion of the initial Cl to the ionic form. Crude V (9 g., obtained by chlorination of 2,3-phenyl-1-indanone according to DeFazi and Banchetti, C.A. 41, 7393f) refluxed 45 min. in 180 ml. 5% alc. KOH, concentrated

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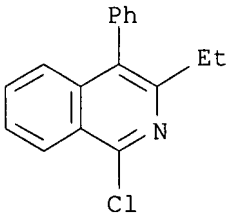
to 45 ml., diluted with H2O, acidified with dilute H2SO4, the cooled product boiled 10 min. in C6H6 over C, and the decolorized filtered solution cooled gave 2.8 g. 2-HO2CC6H4CPh:CPhCl (IX), m. 199-201°, converted (1.0 g.) by successive treatment with SOCl2 and NH3 to 0.85g. I (R = H, R' = Ph) (X), m. 199-201°. The mother liquors from IX diluted with petr. ether yielded 2.7 g. isomeric IX (Xa), m. 159-63°, similarly converted to the isomeric X (Xb), m. 154-6°. IX (1.5 g.) and 1 g. PCl5 heated on a steam bath, the homogeneous solution taken up in C6H6, poured into H2O, the organic layer washed with aqueous Na2CO3 and H2O, and the dried solution concentrated and diluted with petr. ether gave authentic V, converted by boiling 15 min. in MeOH to 2-chloro-3-methoxy-2,3-diphenyl-1-hydrindanone, m. 168-70°. X (0.5 g.) refluxed 1 hr. in 15 ml. 10% KOH in (CH2OH)2 the cooled mixture diluted with H2O, filtered, and the product recrystd. (C6H6-ligroine) gave a compound, C28H24N2O2, m. 240-80° (decomposition, unchanged after sublimation at 1 mm.), also obtained by analogous treatment of Xb. The original aqueous filtrate acidified and extracted with Et2O gave a partially resinous mixture giving a pos. test for BzOH. X (1.5 g.) and 0.8 g. finely powdered NaNH2 refluxed 45 min. in 20 ml. PhMe and the cooled clear yellow solution treated cautiously with H2O to decompose the excess NaNH2, the organic layer concentrated to 10 ml., and the product recrystd. gave 0.8 g. II (R = H, R' = Ph) (XI), m. 250-2°, also similarly obtained from Xb. The stereoisomeric mixture of IX and Xa (2.5 g.) treated with 5 g. SOCl2, the product boiled 10 min. in C6H6 with 2 g. PhNH2, the washed (H2O, dilute HCl, aqueous Na2CO3) and dried (MgSO4) mixture distilled, and the resinous product crystallized (MeOH) gave 1.1 g. I (R = R' = Ph) (XII), m. 199-200°. The mother liquors evaporated to dryness and the residue crystallized (ligroine containing a small proportion of C6H6) gave. 1.4 g. prismatic XII, m. 130-2°. Attempts to cyclize XII with alc. KOH, KOH in (CH2OH)2, and NaNH2 in xylene were unsuccessful and XII was recovered. XI (0.4 g.) and 0.8 g. POCl3 heated 40 min. on a steam bath, the cooled mixture decompd, on ice, made alkaline with NaOH, and the precipitate crystallized (ligroine) gave 0.3 g. 1-chloro-3,4-diphenylisoquinoline, m. 196-7°, hydrogenated (0.2 g.) in alc. with Pd-CaCO3 to yield 0.15 g. III (3-substituent = Ph), m. 155-6°. I (R = H, R' = Me) (1 g.) and 0.5 g. NaNH2 refluxed 30 min. in 10 ml. dry PhMe, the cooled yellow solution treated cautiously with H2O, filtered, the organometallic precipitate boiled 5 min. in 25% HCl, the cooled solution filtered, and the completely organic product (0.7 g.) washed and dried gave authentic II (R = H, R' = Me), m. 280-2°, reduced catalytically to oily III (3-substituent = Me); HCl salt, m. 228-31° (decomposition).

IT 101602-30-6P, Isoquinoline, 1-chloro-3-ethyl-4-phenyl-
102183-41-5P, Isoquinoline, 1-chloro-3,4-diphenyl-
RL: PREP (Preparation)
(preparation of)

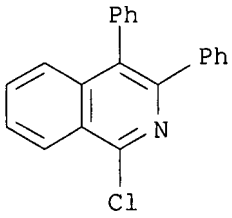
RN 101602-30-6 HCAPLUS

CN Isoquinoline, 1-chloro-3-ethyl-4-phenyl- (6CI) (CA INDEX NAME)

10572342



RN 102183-41-5 HCAPLUS
CN Isoquinoline, 1-chloro-3,4-diphenyl- (6CI, 9CI) (CA INDEX NAME)



L14 ANSWER 29 OF 31 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1958:88105 HCAPLUS
DOCUMENT NUMBER: 52:88105
ORIGINAL REFERENCE NO.: 52:15536f-i,15537a-h
TITLE: New synthesis of 4-phenylisoquinoline and an attempt to prepare 3-phenylisoquinoline
AUTHOR(S): Berti, Giancarlo
CORPORATE SOURCE: Univ. Pisa
SOURCE: Gazzetta Chimica Italiana (1957), 87, 707-19
CODEN: GCITA9; ISSN: 0016-5603
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 52:88105

AB cf. C.A. 47, 4341i. By the action of PCl5 followed by treatment with NH3, 3-methyl-3-phenylphthalide (I) and o-(HO2C)C6H4CPh:CH2 (II) gave o-(H2NCO)C6H4CPh:CHCl (III), cyclized by KOH to 4-phenylisocarbostyryl (IV) and converted to 4-phenylisoquinoline (V). The same series of reactions with 3-benzylphthalide (VI) and o-(HO2C)C6H4CH:CHPh (VII) failed to give the desired 3-phenylisoquinoline. MeMgI (from 16 g. MeI, 2.7 g. Mg, and 100 ml. Et2O) stirred with slow addition of 10 g. o-BzC6H4CO2H in 100 ml. Et2O, the mixture refluxed 1 hr., stored overnight, decomposed with H2SO4 and ice, the Et2O layer washed with aqueous Na2S2O3 and NaOH, the dried extract evaporated, and the product crystallized (C6H6) gave 5 g. I, m. 79-81°. I treated with an equimol. amount of alc. 20% KOH, the solution evaporated, the residue dehydrated at 230°, taken up in H2O, the solution filtered, acidified, and the crude precipitate taken up in aqueous Na2CO3 and repptd. with HCl gave 60-70% II, m. 134-6° (50% AcOH) (cf. Bergmann, C.A. 33, 42257). I (5 g.) and 10 g. PCl5 heated to 100° in 10 min. and to 140° in 1 hr., the residue taken up in C6H6, the solution washed with aqueous Na2CO3 and saturated NaCl

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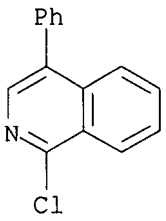
solution, dried over CaCl2 saturated 15 min. with dry NH3, filtered from NH4Cl, and the concentrated filtrate diluted with petr. ether gave 2.7 g. III, m. 141-3° (petr. ether-CHCl3), also obtained by a similar procedure from II. III (2 g.) in 10 ml. 10% KOH in HO(CH2)2OH heated 1 hr. at 150°, cooled, and diluted with H2O gave 1 g. IV, m. 208-17°, converted by heating 15 min. at 100° with 2 parts POCl3, decomposing with ice, and alkalinizing with NaOH to 1-chloro-4-phenylisoquinoline (VIII), m. 117-18° (ligroine). III (0.25 g.) and 0.25 g. CrO3 in 8 ml. AcOH heated 30 min. at 100°, the cooled mixture taken up in Et2O, and the washed and dried extract evaporated gave the known o-BzC6H4CONH2, m. 158-60°(PhMe). VIII (0.18 g.) in 20 ml. alc. treated with 4 ml. 10% alc. KOH and 0.4 g. PdO2-CaCO3, hydrogenated 40 min., the mixture filtered (CO2 atmospheric), and the filtrate evaporated gave 0.12 g. V, m. 80-1° (dilute alc.); picrate, m. 208-10° (PhMe) (cf. Krabbe, et al., C.A. 32, 21253). Treatment of VI and analogous benzylidene compound with PCl5 gave 3-(α-chlorobenzylidene)phthalides and 3-chloro-3-(α-chlorobenzyl)phthalides. The presence of the H atom in position 3 seems to be incompatible with the production of the acid chloride. Accordingly, the above series of transformations was attempted with VII. VII (1 g.) and 2 g. PCl5 heated 30 min. at 100°, the cooled mixture diluted with C6H6 and H2O, the C6H6 layer washed with aqueous NaHCO3, filtered through a filter moistened with C6H6, the filtrate saturated 10 min. with dry NH3, and the product washed with H2O gave 0.5 g. o-H2NCOC6H4CH:CHPh (IX), m. 190-2° (cf. C.A. 50, 12929a). Working up the C6H6 filtrate gave 0.2 g. 4-chloro-3-phenyl-3,4-dihydroisocoumarin (X), m. 106-10°. VII (7 g.) and 13.5 g. PCl5 heated to 135° in 15 min., the temperature increased slowly to 160° in 1 hr. with distillation of 8.2 g. mixture of PCl3 and POCl3, the oily residue taken up in C6H6, the washed and dried solution saturated 30 min. with dry NH3, and the precipitate washed with H2O and crystallized (CHCl3-CCl4 and C6H6) gave 2.5 g. o-PhCHClCHClC6H4CONH2 (XI), m. 146-8°, and a small amount IX. The initial C6H6 filtrate evaporated and the residue crystallized (MeOH and C6H6-ligroine) yielded 1 g. X. VII (2 g.) in 30 ml. CHCl3 saturated 30 min. with dry Cl, the solution washed with aqueous Na2CO3, dried over MgSO4, evaporated, and the residue recrystd. (C6H6-ligroine) gave 1.85 g. X. Chlorination under various conditions gave invariably X and never the o-HO2CC6H4CHClCHClPh. X (0.2 g.) heated in a metal bath to 250° and the residue crystallized from a small volume of alc. and from ligroine yielded 3-phenylisocoumarin, m. 89-90°, converted by boiling with concentrated NaOH and acidification of the cooled solution to o-BzCH2C6H4CO2H, m. 160° (decomposition). X (0.6 g.) in 30 ml. alc. hydrogenated 45 min. with 0.15 g. 5% Pd-C at 20°/760, the mixture filtered, the filtrate evaporated, the residue extracted with aqueous Na2CO3, filtered, and the alkali-insol. residue crystallized (dilute alc.) gave authentic 3-phenyl-3,4-dihydroisocoumarin, m. 89-90°. The alkaline filtrate acidified, filtered, and the mixture of crude acids (0.25 g.) containing Cl twice recrystd. (C6H6-ligroine) gave needles of o-PhCH2CH2C6H4CO2H, m. 129-30°; amide, m. 128°, produced by reduction of IX with 5% Pd-C or by similar reduction of IX. XI (1.4 g.) heated 6 min. at 150-60°/14, the yellow residue extracted twice with 20 ml. C6H6, and the insol. material crystallized (AcOH) gave 0.85 g. mixture (XII) of 3-benzylidene-1-imino-1,3-dihydroisobenzofuran and 1-imino-3-phenyl-2,1H-benzopyran HCl salts, m. 210-15° (decomposition). XII (0.3 g.) heated 15 min. in 10 ml. N HCl at 100° and the cooled mixture

filtered gave 0.2 g. VI (alc.). The alc. mother liquor boiled 5 min. with NaOH, the solution diluted with H2O, acidified, filtered, and the precipitate crystallized (dilute alc.) yielded o-BzCH2C6H4CO2H (XIII), m. 160-2°. XII (0.3 g.) taken up in 2N NaOH, the mixture kept several hrs. at room temperature, filtered, and the residue crystallized (alc.) gave 0.1 g. o-BzCH2C6H4CN (XIIIa), m. 109-11°. Acidification of the filtrate and crystallization of the precipitate (alc.) yielded 3-benzylidenephthalimidine (XIV), m. 181°. XIIIa (0.1 g.) in 2 ml. anhydrous MeOH saturated with dry HCl, poured into H2O, the solution heated on a steam bath 10 min., cooled, extracted with Et2O, the extract evaporated, the residue taken up in 3 ml. N alc. KOH, boiled 10 min., diluted with H2O, extracted with Et2O, the aqueous solution acidified, filtered when cool, and the product crystallized gave XIII. XI (0.5 g.) in 15 ml. alc. and 10 ml. 8% alc. KOH boiled 4 min. and diluted with H2O gave 0.35 g. o-PhCH:CClC6H4CONH2, m. 134-6° (C6H6-ligroine). XI (1 g.) in 50 ml. 10% alc. KOH refluxed 2 hrs. and poured into H2O gave 0.7 g. Cl-free product, crystallized (alc. and C6H6-ligroine) to give 0.15 g. XIV. Working up the mother liquors yielded a mixture of products, C15H11NO.

IT 65810-96-0P, Isoquinoline, 1-chloro-4-phenyl-
RL: PREP (Preparation)
(preparation of)

RN 65810-96-0 HCAPLUS

CN Isoquinoline, 1-chloro-4-phenyl- (6CI, 9CI) (CA INDEX NAME)



L14 ANSWER 30 OF 31 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1953:66025 HCAPLUS

DOCUMENT NUMBER: 47:66025

ORIGINAL REFERENCE NO.: 47:11202a-i,11203a-i,11204a-i,11205a-d

TITLE: Isoquinoline derivatives as local anesthetics

AUTHOR(S): Anderson, Elvin L.; Wilson, James W.; Ullyot, Glenn E.

CORPORATE SOURCE: Smith, Kline, and French Labs., Philadelphia, PA

SOURCE: Journal of the American Pharmaceutical Association, Scientific Edition (1952), 41, 643-50
CODEN: JAPMA8; ISSN: 0095-9553

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

AB cf. C.A. 45, 42712. Various 1-(aminoalkoxy)isoquinoline derivs. and the appropriate 1-chloroisoquinoline intermediates are described. The effect of structural variations is reported. In general, local anesthetic activity was maximum when the isoquinoline was substituted in the 3-position by a Bu group and in the 1-position by a (1-methyl-3-piperidyloxy) group. Increasing the size of the 3-alkyl substituent was without effect. Further modification of this group, such as branching or the substitution of aryl or aralkyl groups, decreased the activity, as did also alterations

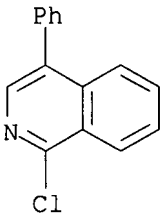
of the basic side-chain. In general, the dimethylaminoethoxy side-chain was the most effective of nonheterocyclic structures. Replacement of the O ether linkage with either S or N lowered the activity. The introduction of alkyl, alkoxy, amino, acetamido, or halo groups, not only lowered the activity, but increased the toxicity and irritation. The required amino alcs. were prepared by known methods. Thus, 2,2,4,6-tetramethyl-1-piperidineethanol, b11 126-8°, nD23 1.4817, was prepared from 2,2,4,6-tetramethylpiperidine and ClCH2CH2OH. 2-Hexyl-1-piperidineethanol b0.3 100-4° (nD23 1.4760). Most of the intermediate substituted isoquinolones were prepared from (1) the appropriate 1-amino-1-(3-phthalidyl)alkanes or (2) by cyclization of phenethyl isocyanates with AlCl3 to tetrahydroisoquinolones followed by dehydrogenation. Thus, Et 3,4-dimethoxyphenethylcarbamate (I), b4 176-8°, was prepared by treating 181 g. (1 mole) of 3,4-(MeO)2C6H3CH2CH2NH2 in 250 cc. dry C6H6 with 54.5 g. (0.5 mole) ClCO2Et in 100 cc. dry C6H6 over 45 min. at 50° with stirring, stirring 30 min. at 50°, extracting the mixture with H2O, then with saturated NaHCO3 solution, distilling off the C6H6, and distilling the residue I (51 g.) (0.2 mole) was gently refluxed 3 hrs. with 100 g. (0.7 mole) POCl3 and 7 g. P2O5, the mixture hydrolyzed with ice, made alkaline with excess 40% NaOH, and the product extracted with CHCl3, and recrystd. from MeCOEt, giving 6,7-dimethoxy-3,4-dihydro1(2H)-isoquinolone (II). II (2 g.) and 0.3 g. 30% Pd-C catalyst heated from 200° to 240° over 30 min. while dry N was bubbled into the mixture gave 6,7-dimethoxy-1(2H)isoquinolone, m. 237-8° (from CHCl3). (PhCH2)2CHNH2, prepared from (PhCH2)2CO by the Leuckart reaction, was converted with COCl2 in PhNO2 to 2,2-diphenylisopropyl isocyanate (III), b15 197°, which with NH3 gave the unsym. urea, m. 138-8.5°. A mixture of 28 g. (0.08 mole) AlCl3 in 150 cc. PhNO2 and 20 g. (0.08 mole) III stirred 3 hrs. at 75°,allowed to cool, poured slowly into 250 cc. ice water, the whole extracted with CHCl3, and the solvents distilled in vacuo gave 3-benzyl-3,4-dihydro-1(2H)-isoquinolone (IV), m.148-8.5° (from dilute EtOH). Dehydrogenation of IV 6 hrs. at 305-20° gave 3-benzyl-1(2H)-isoquinolone, m. 192-3° (from iso-PrOH). p-BuC6H4CH2Cl with KCN gave p-BuC6H4CH2CN (V), b19 163-5°, nD23 1.5061, hydrolyzed with 50% H2SO4 to p-BuC6H4CO2H, m. 73-4.5° (from dilute EtOH). V (112 g.) in 725 cc. MeOH saturated with NH3 reduced over Raney Ni at room temperature and an initial pressure of 1420 lb./sq. in., gave 92% (p-butylphenethylamine) (VI), b20 146-51°, nD24 1.5105-1.5132; VI.HCl m. 184-5.5°. VI with COCl2 yielded 92% p-butylphenethyl isocyanate (VII), b16 150-6°, nD24 1.5060-1.5068. Cyclization of VII by AlCl3 as above gave 7-butyl-3,4-dihydro-1(2H)-isoquinolone, b0.5 180-3°; nD24 1.5545, m. 45-6°, dehydrogenated to 7-butyl-1(2H)-isoquinolone, m. 127.5-9° (from dilute EtOH). Treatment of p-MeOC6H4CH2CHMeNH2 with COCl2 yielded the isocyanate, b3 112-13°, nD23 1.5168, which gave with concentrated NH4OH, presumably the urea derivative, m. 169-70° (from dilute EtOH). Cyclization of the isocyanate, with the temperature kept at 45°, yielded 3-methyl-7-methoxy-3,4-dihydro-1(2H)-isoquinolone, m. 149-50° (from iso-PrOH). Dehydrogenation 4 hrs. at 250-60° gave 3-methyl-7-methoxy-1(2H)-isoquinolone, m. 140-1° (from EtOH). The 1-chloroisoquinolines were obtained from the isoquinolones with POCl3 or from the appropriate isoquinoline N-oxide or N-oxide-HCl with POCl3. The position of the entering Cl was established as follows: 1-chloro-3-ethylisoquinoline (VIII) dehalogenated over Raney Ni gave 3-ethylisoquinoline (IX); picrate, 173-3.5° (reported 171-2°). IX treated with H2O2 and AcOH gave 3-ethylisoquinoline N-oxide-HCL, m. 203-3.5°, and the N-oxide with POCl3 gave VIII which, when refluxed with dilute H2SO4, yielded 3-ethyl-1(2H)-isoquinolone,

m. 139-140°, alone and with an authentic sample. 3-Methyl-4-butylisoquinoline N-oxide-HCl(prepared by H2O2-AcOH oxidation of the isoquinoline), m. 196-8°. 3-Methyl-4-propylisoquinoline N-oxide (X), m. 114-15°; X.HCl, m. 212-15°. The aminoalkyl ethers were prepared as previously described. The following x-substituted 1-chloroisoquinolines [yields (%) in parentheses] were prepared: 3-iso-Bu, b0.3 125-6°, nD23 1.5841 (73); 3-Am, b2 142-4°, nD24 1.5874 (78); 3-hexyl, b0.3 151-3°, nD23 1.5701 (62); 3-Ph, m. 76-8° (81); 4-Ph, m. 114-15.5° (100); 3-PhCH2, b0.5 180-2°, nD23 1.6642 (74); 4-Br, m. 97.5-8° (85); 5-O2N, m. 183-4° (57); 5-H2N, m. 175-6° (77); 3,5-Et(O2N), m. 92.5-3.5° (89); 3,5-Et(H2N), m. 124-5° (83); 7-Bu, b0.5 134-6°, nD23 1.5872 (85); 6,7-(MeO)2, m. 155-60° (-) (picrate, m. 190-1°); 3,7-Me(MeO), m. 111-12° (39); 3,6,7-EtMe2, b2.5 155-6°, nD25 1.6050 (33) (picrate m. 114.5-15°); 3,4-MePr, b1.5 143-5°, nD20 1.6005 (78); 3,4-MeBu, b2 158-60°, nD28 1.5874 (51); 3,7-Et(H2N), m. 145-5.5° (73).

IT 65810-96-0P, Isoquinoline, 1-chloro-4-phenyl-
RL: PREP (Preparation)
(preparation of)

RN 65810-96-0 HCAPLUS

CN Isoquinoline, 1-chloro-4-phenyl- (6CI, 9CI) (CA INDEX NAME)



L14 ANSWER 31 OF 31 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1953:25387 HCAPLUS
DOCUMENT NUMBER: 47:25387
ORIGINAL REFERENCE NO.: 47:4341h-i,4342a-f
TITLE: A new method of synthesis of derivatives of isoquinoline. A preliminary note
AUTHOR(S): Berti, Giancarlo
CORPORATE SOURCE: Univ. Pisa, Italy
SOURCE: Gazzetta Chimica Italiana (1951), 81, 868-74
CODEN: GCITA9; ISSN: 0016-5603
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 47:25387

GI For diagram(s), see printed CA Issue.

AB Treatment of certain amides of o-PhCH2CCl:CHC6H4CO2H (I) with KOH eliminates 1 HCl mol. and results in cyclization involving the o-C-CC6H4C-N group, with formation of derivs. of iso-carbostyril. This reaction is of great interest because it represents a wholly new method of synthesis of the bicyclic isoquinoline (II) system and makes possible the preparation of complex derivs. of II. 3-Ethyl-3-phenylphthalide (III) (2 g.) and 4 g. PCl5, heated 1 hr. at 120°, diluted with C6H6, poured into ice water, agitated 1 min., the C6H6 solution washed with cold aqueous Na2CO3, the C6H6 solution filtered, NH3 gas passed through for 30 min., the mixture filtered, concentrated, ligroine added, and the precipitate (1.2 g.) purified by MeOH

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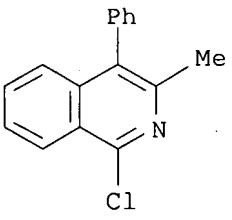
or ligroine-C6H6, yields the amide, C16H14ONCl (IV), of I, m. 135-6°. A smaller yield is obtained by adding concentrated NH4OH to the acid chloride (V), in C6H6 and boiling off the C6H6. A solution of V (from 1 g. III) treated with 2 g. MeNH3Cl, 20% aqueous NaOH added dropwise, the C6H6 layer washed with dilute HCl, concentrated, diluted with ligroine, and the precipitate (0.6 g.) purified by aqueous EtOH, yields the N-methylamide, C17H16ONCl (VI), of I, m. 148-52°. It is a mixture of 2 isomers, with that corresponding to the acid m. 194-5° in the major proportion. IV (0.8 g.) in 10 cc. 10% alc. KOH, refluxed 4 hrs. (KCl ppts.), diluted with water, and the precipitate purified by C6H6, yields 0.6 g. of 3-methyl-4-phenyliso-carbostyril (VII), m. 292-4°. VII (0.3 g.) and 0.2 g. POCl3, refluxed 30 min., poured into ice water, made alkaline with NaOH, extracted with Et2O, the extract evaporated, and the residue purified by hot EtOH, yield 0.27 g. 1-chloro-3-methyl-4-phenylisoquinoline (VIII), m. 100-101°. VIII (0.5 g.), 0.3 g. red P, and 3.5 cc. HI (b. 127°), heated 3 hrs. in a sealed tube at 165-70°, taken up in boiling water, filtered hot, the filtrate made alkaline with NaOH, and the flocculent oily precipitate dissolved in aqueous HCl and repptd. by NaOH, yield 3-methyl-4-phenylisoquinoline (IX), ultraviolet absorption maximum in EtOH 270, 315, and 331 mμ (maximum of isoquinoline 267, 305, and 318); hence the bathochromic effect of the Ph group is evident. An aqueous suspension of IX extracted with C6H6, the extract evaporated, the residue taken up in EtOH, alc. picric acid added, the solution concentrated, and the precipitate purified by EtOH, yields the picrate, C16H13N.C6H3O7N3, m. 195°. o-PhCH2CCl:CHC6H4CONHPh (X) (0.356 g.) and 12 cc. 8% alc. KOH, refluxed 3 hrs., water added, and the precipitate purified by MeOH, yield 0.302 g. of 2,4-diphenyl-3-methylisocarbostyril (XI), m. 222-4°. Titration with AgNO3 of the dilute alc. solution before purification indicated a 93% yield of XI. XI is formed from both forms of X, m. 120-1° and 143-5° (cf. Freiser and Glowacki, C.A. 43, 5784c). VI (0.5 g.) and 10 cc. 10% alc. KOH, refluxed 3 hrs. (KCl seps.), diluted with water, and the precipitate (0.42 g.) purified by MeOH, yield 2,3-dimethyl-4-phenylisocarbostyril, C6H4.CO.NMe.CMe:CPh, m. 214-15°. Titration of the solution indicated an 80% yield. The only drawback at present to this method of synthesis is the preparation of the substituted o-(2-chlorovinyl)benzoic acids, only 3 of which have been described and low yields reported. However, recent work (cf. de Fazi and Carboni, C.A. 43, 2610e; D. and B., C.A. 44, 7298c; B., C.A. 46, 5015e) gives promise of surmounting this difficulty.

IT 101423-02-3P, Isoquinoline, 1-chloro-3-methyl-4-phenyl-
RL: PREP (Preparation)
(preparation of)

RN 101423-02-3 HCAPLUS

CN Isoquinoline, 1-chloro-3-methyl-4-phenyl- (6CI) (CA INDEX NAME)



Updated Search

10572342

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=> file caold
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                    189.51     717.04

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                    -25.74     -26.52

FILE 'CAOLD' ENTERED AT 01:35:35 ON 20 SEP 2007
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FILE COVERS 1907-1966
FILE LAST UPDATED:  01 May 1997 (19970501/UP)

  This file contains CAS Registry Numbers for easy and accurate
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  assignees, and patent information, e.g., patent numbers, are
  now searchable from 1907-1966.  TIFF images of CA abstracts
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=> d his

     (FILE 'HOME' ENTERED AT 01:26:17 ON 20 SEP 2007)

     FILE 'REGISTRY' ENTERED AT 01:26:30 ON 20 SEP 2007
L1             STRUCTURE UPLOADED
L2           0 S L1
L3           1 S L1 FULL

     FILE 'HCAPLUS' ENTERED AT 01:29:18 ON 20 SEP 2007
L4           1 S L3

     FILE 'CAOLD' ENTERED AT 01:29:31 ON 20 SEP 2007
L5           0 S L3

     FILE 'REGISTRY' ENTERED AT 01:29:39 ON 20 SEP 2007
L6             STRUCTURE UPLOADED
L7           0 S L6
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L9             STRUCTURE UPLOADED
L10          7 S L9
L11         78 S L9 FULL

     FILE 'HCAPLUS' ENTERED AT 01:32:04 ON 20 SEP 2007
L12         33 S L11
L13          2 S L12 AND TROTTER, B?/AU
L14         31 S L12 NOT L13
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Updated Search

10572342

L15 0 S L14 AND NANDA, K?/AU
L16 0 S L14 AND KETT, N?/AU
L17 0 S L14 AND DINSMORE, C?/AU
L18 0 S L14 AND PONTICELLO, G?/AU
L19 0 S L14 AND CLAREMON, D?/AU

FILE 'CAOLD' ENTERED AT 01:35:35 ON 20 SEP 2007

=> s l11
L20 3 L11

=> d l20, all, 1-3

L20 ANSWER 1 OF 3 CAOLD COPYRIGHT 2007 ACS on STN
AN CA54:14934f CAOLD
TI ultraviolet spectra of derivs. of 3- and 4-phenylisoquinoline
AU Berti, Giancarlo; Corti, P.
IT 491-30-5 1741-39-5 3681-64-9 4581-48-0 4581-49-1
4666-81-3 4677-87-6 7115-13-1 16769-57-6 19571-30-3 31538-72-4
36828-24-7 37993-76-3 52839-45-9 55150-54-4 65810-96-0
91426-59-4 93119-96-1 98089-17-9 101423-02-3
101602-30-6 102183-41-5 102466-77-3 108979-41-5
108981-22-2

L20 ANSWER 2 OF 3 CAOLD COPYRIGHT 2007 ACS on STN
AN CA53:20063a CAOLD
TI synthesis of isoquinoline derivs.
AU Berti, Giancarlo; Corti, P.
IT 496-10-6 40182-22-7 52839-45-9 53133-95-2 93119-96-1
98089-17-9 101571-14-6 101602-30-6 102183-41-5
102451-79-6 102466-63-7 102467-48-1 102590-56-7 103035-62-7
108979-41-5 114795-39-0

L20 ANSWER 3 OF 3 CAOLD COPYRIGHT 2007 ACS on STN
AN CA52:15536f CAOLD
TI synthesis of 4-phenylisoquinoline and an attempt to prepare
3-phenylisoquinoline
AU Berti, Giancarlo
IT 2674-44-4 2881-31-4 4809-08-9 4890-85-1 5194-47-8
10517-64-3 17582-84-2 18019-56-2 19571-30-3 36795-31-0
36828-24-7 37993-76-3 63404-82-0 65810-96-0 100865-28-9
100954-88-9 101096-27-9 109365-99-3 110155-83-4

=> FIL REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
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CA SUBSCRIBER PRICE	0.00	-26.52

FILE 'REGISTRY' ENTERED AT 01:35:54 ON 20 SEP 2007
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STRUCTURE FILE UPDATES: 18 SEP 2007 HIGHEST RN 947490-11-1
DICTIONARY FILE UPDATES: 18 SEP 2007 HIGHEST RN 947490-11-1

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http://www.cas.org/support/stngen/stndoc/properties.html

=> S 65810-96-0/RN

L21 1 65810-96-0/RN

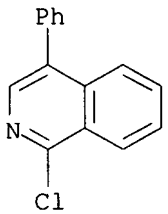
=> SET NOTICE 1 DISPLAY

NOTICE SET TO 1 U.S. DOLLAR FOR DISPLAY COMMAND
SET COMMAND COMPLETED

=> D L21 SQIDE 1-

YOU HAVE REQUESTED DATA FROM 1 ANSWERS - CONTINUE? Y/(N):y
THE ESTIMATED COST FOR THIS REQUEST IS 6.55 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L21 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN
RN 65810-96-0 REGISTRY
CN Isoquinoline, 1-chloro-4-phenyl- (6CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN 1-Chloro-4-phenylisoquinoline
MF C15 H10 Cl N
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); NORL (No role in record)



Updated Search

10572342

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

6 REFERENCES IN FILE CA (1907 TO DATE)
6 REFERENCES IN FILE CAPLUS (1907 TO DATE)
2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> SET NOTICE LOGIN DISPLAY

NOTICE SET TO OFF FOR DISPLAY COMMAND
SET COMMAND COMPLETED

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=> FIL REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.40	721.96

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-26.52

FILE 'REGISTRY' ENTERED AT 01:36:09 ON 20 SEP 2007
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STRUCTURE FILE UPDATES: 18 SEP 2007 HIGHEST RN 947490-11-1
DICTIONARY FILE UPDATES: 18 SEP 2007 HIGHEST RN 947490-11-1

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=> S 101423-02-3/RN

L22 1 101423-02-3/RN

=> SET NOTICE 1 DISPLAY

NOTICE SET TO 1 U.S. DOLLAR FOR DISPLAY COMMAND
SET COMMAND COMPLETED

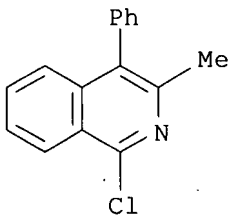
Updated Search

10572342

=> D L22 SQIDE 1-

YOU HAVE REQUESTED DATA FROM 1 ANSWERS - CONTINUE? Y/(N):y
THE ESTIMATED COST FOR THIS REQUEST IS 6.55 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L22 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN
RN 101423-02-3 REGISTRY
CN Isoquinoline, 1-chloro-3-methyl-4-phenyl- (6CI) (CA INDEX NAME)
MF C16 H12 Cl N
SR CAOLD
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS
(*File contains numerically searchable property data)
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation); NORL (No role in record)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> SET NOTICE LOGIN DISPLAY

NOTICE SET TO OFF FOR DISPLAY COMMAND
SET COMMAND COMPLETED

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=> FIL REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.40	724.36

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-26.52

FILE 'REGISTRY' ENTERED AT 01:36:27 ON 20 SEP 2007
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DICTIONARY FILE UPDATES: 18 SEP 2007 HIGHEST RN 947490-11-1

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http://www.cas.org/support/stngen/stndoc/properties.html

=> S 101602-30-6/RN

L23 1 101602-30-6/RN

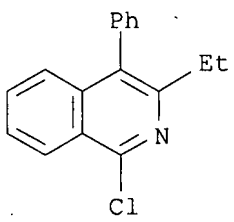
=> SET NOTICE 1 DISPLAY

NOTICE SET TO 1 U.S. DOLLAR FOR DISPLAY COMMAND
SET COMMAND COMPLETED

=> D L23 SQIDE 1-

YOU HAVE REQUESTED DATA FROM 1 ANSWERS - CONTINUE? Y/(N):y
THE ESTIMATED COST FOR THIS REQUEST IS 6.55 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L23 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN
RN 101602-30-6 REGISTRY
CN Isoquinoline, 1-chloro-3-ethyl-4-phenyl- (6CI) (CA INDEX NAME)
MF C17 H14 Cl N
SR CAOLD
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS
(*File contains numerically searchable property data)
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation); NORL (No role in record)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

Updated Search

10572342

2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> SET NOTICE LOGIN DISPLAY

NOTICE SET TO OFF FOR DISPLAY COMMAND
SET COMMAND COMPLETED

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Updated Search